

Hard-Ball Gas as Hard Nut of Statistical Mechanics (why mathematicians missed $1/f$ -noise there)

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We continue discussion of hard-ball models of statistical mechanics, by example of random walk of hard ball immersed into equilibrium ideal gas. Our goal is to highlight decisive role of specific phase-space subsets, despite their vanishingly small Lebesgue measures under the Boltzmann-Grad limit. The “art of draining” such subsets in conventional mathematical constructions resulted in loss of so principal property of many-particle systems as $1/f$ -noise in diffusivities, mobilities and other transport and relaxation rates. We suggest new approaches to formulation and analysis of evolution equations for hierarchy of probability distribution functions of infinite hard-ball systems, thus further overcoming prejudices of Boltzmannian kinetics and mistakes of its modern adepts.

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I. INTRODUCTION

1. A system of (infinitely) many elastic rigid, or hard, balls (hard spheres) is attractive model of classical gases with short-range repulsive interactions. Especially, - as many do believe, - for desired rigorous derivation of celebrated Boltzmann’s kinetic equation (BE) under the Boltzmann-Grad limit (BGL). Most significant results of the corresponding mathematical activity are collected in monograph [1] and earlier review article [2].

Unfortunately, these results are in contradiction to theoretical analysis performed in [3], moreover, to the N. Krylov’s fundamental criticism [4] of prejudices acclimatized in statistical mechanics. These works pointed out why BE has no chances to be valid even under BGL.

The essence of this contradiction is very simple. On one hand, BE declares a priori definite differential cross-section of collisions presuming that they obey uniform (probability) distribution over impact parameter values. On the other hand, in reality there are no physical mechanisms to enforce collisions of any given particle to build up some smooth distribution, all the more a priori predictable one [3, 5]. Hence, there are no physical grounds for thinking in terms of imaginary a priori “cross-sections” or “probabilities” of (various sorts of) collisions, or other beforehand established characteristics of time rates of random events [4]).

2. Such radical controversy between two ways of thinking about the same things says that one of them stands on wrong concept or postulate. Below, we shall argue once again that it is the Boltzmann molecular chaos paradigm. It seems so doubtless that itself provokes mistakes in attempts of its mathematical substantiation expounded in [1, 2]. More precisely, formal methods exploited in [1, 2] (such as artificial filtration of initial conditions and term-by-term consideration of BGL of infinite iteration series) ignore the fact that actual

dynamical roles of different many-particle configurations (clusters and events) are not proportional to their native (Lebesgue or Gibbs) probability measures. As the consequence, many important factors were missed there.

By these reasons, below we suggest new visual illustrations of statistical significance of non-typical (“improbable”) many-particle configurations, even in BGL, hence, existence of strong statistical correlations between their constituting particles.

3. Some of defects of conventional formalism are implied by ambiguities in its probability-theoretical formulation of the hard-ball collision rules. The matter is that conventional formulation treats collisions like instant states, instead of events with non-zero, let small, duration. This, in turn, implies neglecting above mentioned “improbable” configurations and eventually loss of “lion’s share” of theory’s physical meaning.

On account of all that, below we suggest an alternative probability-theoretical representation of hard-ball collisions, by introducing them as limit case of interactions via continuous potentials. The corresponding non-standard treatment of hard-ball limit of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy of equations is fully consistent with more general considerations [3, 5].

This approach, as well as some other original tricks and approaches suggested below, help to realize that kinematic possibility of collisions is sufficient reason for appearance of statistical correlations between related particles. This insight can prevent at least a part of wrong hypotheses about “independence” of random events..

4. For brevity and simplicity, we shall concentrate mainly on special but principally important problem of (hard-ball) “molecular Brownian particle” in thermodynamically equilibrium ideal gas. At that, we use some designations and definitions from preprints [6, 7] where hard-ball systems already were under our attention.

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II. BASIC PROPERTIES OF RIGID ELASTIC COLLISIONS AND QUESTION OF THEIR STATISTICAL DESCRIPTION

A. Hard-ball collision rules

Undoubtedly, in Hamiltonian statistical mechanics this rule must establish that total momentum of pair of particles, - let with masses m and M , - conserves under their collision, $P + p = P^* + p^*$, while their relative velocity $u = v - V$ (with $v = p/m$ and $V = P/M$ being individual velocities) changes according to

$$\Omega \cdot u = -\Omega \cdot u^* , \quad (1)$$

with Ω denoting unit vector ($\Omega = \rho/|\rho|$, $|\Omega| = 1$) parallel to radius-vector $\rho = r - R$ connecting centers of the particles at *perigee* of collision. Specificity of hard balls is that there $|\rho| = a = \text{const}$ regardless of $|u|$, so that at the *perigee* always $\rho = a\Omega$. At that, tangential component of u conserves as usually,

$$(1 - \Omega \otimes \Omega) u = (1 - \Omega \otimes \Omega) u^* , \quad (2)$$

and Ω together with u give complete kinematic characterization of the collision in itself.

B. Conventional probability-theoretical representation of hard-ball collision rules

In statistical mechanics, in place of kinematic and dynamic characteristics of particles' motion one has their "statistical ensembles" and deals with probability distribution functions (DF).

If elastic collision of hard balls is thought of as an "instant event" consuming neither time nor space, then it seems natural to represent it by boundary condition for a DF, let $F(\cdot)$, as follows:

$$F(\rho = a\Omega, u) = F(\rho = a\Omega, u^*) , \quad (3)$$

where u and u^* are interpreted as relative velocities "before" and "after" collision (or vice versa) satisfying relations (1)-(2).

This is basic prescription of conventional formal construction of hard-ball statistical mechanics (SM) [1, 2].

C. Confusions of conventional probability-theoretical description of hard-ball collisions

Common beliefs in physical adequacy of the condition (3) in fact is beneath criticism and can be easily destroyed.

1. Indeed, first of all, let relative velocity before a collision is strictly definite, $u = u_0$ (with $\Omega \cdot u_0 < 0$), so that in respect to it some DF looks like delta-function. Without loss of generality, we can require its normalization to unit. Then, involving also outcome of the collision and following condition Eq.3, we have to write

$$F(\rho = a\Omega, u) = \delta(u - u_0) + \delta(u - u_0^*)$$

This expression, however, evidently violates the normalization. Therefore it should be manually changed to

$$F(\rho = a\Omega, u) = \frac{1}{2} \delta(u - u_0) + \frac{1}{2} \delta(u - u_0^*)$$

It thus shows that the Eq.3, under properly corrected interpretation, represents particles which are "by half before" and "by half after" collision.

2. This observation reminds that any real collision is not an instant state but a process, or "event", more or less extended in space and time. In other words, it includes relative motion of colliding particles which, therefore, falls out from motion of collision as the whole.

Consequently, spatial distribution of number density of collision events drifts with centre of mass velocity $(MV + mv)/(M + m)$. This circumstance, in turn, inevitably implies violation of Boltzmann's molecular chaos, in the form of 1/f-noise in diffusivities (mobilities) of gas particles [3].

Taking into account non-vanishing duration of collisions, and considering them in the centre of mass (CM) frame, we may rewrite the condition (3) as

$$F(\rho = a\Omega - u dt, u) = F(\rho = a\Omega + u^* dt^*, u^*) , \quad (4)$$

with an infinitesimal $dt > 0$ and $dt^* > 0$. Clearly, this condition, in addition to (3), prescribes also

$$- [u \cdot \nabla_\rho F(\rho, u)]_{|\rho|=a} = [u^* \cdot \nabla_\rho F(\rho, u^*)]_{|\rho|=a} = 0 \quad (5)$$

It just means that relative motion of particles is inner part of collision's constitution and thus is excluded from particles' drifts (flights) during collision [7].

3. To continue our critical remarks, notice that from physical viewpoint, strictly speaking, there is no necessity to identify u and u^* in (3) with "initial" and "final" values of relative velocity (before and after collision). Instead, one has rights to interpret $F(\rho = a\Omega, u)$ in (3) as probability distribution of intermediate values of relative velocity which can be found in the course of collision ("inside collision").

Such vision naturally appears, for instance, when considering hard-ball limit of BBGKY equations. Let us illustrate how it does.

III. ALTERNATIVE (NON-CONVENTIONAL) PROBABILITY-THEORETICAL FORMULATION OF HARD-BALL COLLISION RULES

A. Derivation of alternative formulation

Highlighting, as above, and writing out variables of only one pair of interacting particles, we may symbolize evolution of a DF $F(\cdot)$ by equation

$$\begin{aligned} \dot{F}(t, \dots \mathcal{E}, \rho, P, p \dots) = \\ = [\dots - u \cdot \nabla_\rho + \Phi'(\rho) \cdot (\nabla_p - \nabla_P) \dots] \times \\ \times F(t, \dots \mathcal{E}, \rho, P, p \dots), \end{aligned} \quad (6)$$

where $\mathcal{E} = \Phi(\rho) + P^2/2M + p^2/2m$ is energy of the pair, $\Phi(\rho)$ is interaction potential, to be short-range, repulsive and spherically symmetric ($\Phi(\rho) = \Phi(|\rho|)$), and $\Phi'(\rho) = \nabla_\rho \Phi(\rho)$ is interaction force.

The dots in Eq.6 replace omitted terms of evolution operator (in square brackets), the pair's centre of mass position $(MR + mr)/(M + m)$ and "extra particles" variables.

At the same time, we advisedly introduced argument \mathcal{E} , as if it was independent on others, in order to get possibility to treat the DF $F(\cdot)$, - even at arbitrary sharp $\Phi(\rho)$, - as a smooth function of the partial argument ρ in itself. The smoothness means naturally that

$$\frac{|u \cdot \nabla_\rho F(\cdot)|}{F(\cdot)} < \infty, \quad (7)$$

where gradient ∇_ρ does not act onto \mathcal{E} .

The hard-ball interaction results from infinitely sharp potential when

$$\begin{aligned} \Phi(\rho) &\Rightarrow \infty \quad \text{if } |\rho| < a, \\ \Phi(\rho) &\Rightarrow 0 \quad \text{if } |\rho| \geq a \end{aligned} \quad (8)$$

We thus take in mind a sequence of system's evolutions corresponding to sequence of interaction potentials tending to the hard-ball one. At that, we require that at any of these evolutions any DF $F(\cdot)$ stays a smooth function of the evolution time as well (except, may be, very initial stage of evolution, but certainly at late enough "kinetic" stage, in Bogolyubov's terminology [8]). This means that, similarly to (7),

$$\frac{|\partial_t F(\cdot)|}{F(\cdot)} < \infty \quad (9)$$

Then from Eq.6, together with identity

$$[-u \cdot \nabla_\rho + \Phi'(\rho) \cdot (\nabla_p - \nabla_P)] \mathcal{E}(\rho, P, p) = 0,$$

it follows that necessary boundedness

$$\frac{\Phi'(\rho) \cdot (\nabla_p - \nabla_P) F(\cdot)}{F(\cdot)} \Rightarrow \gamma(\cdot) \neq \infty \quad (10)$$

also takes place under limit transition (8), with differentiation operators (momenta gradients), ∇_p and ∇_P , acting on the $F(\cdot)$'s momentum arguments in themselves only (i.e. not touching \mathcal{E}).

Clearly, all this means that under the transition

$$\frac{\Omega \cdot (\nabla_p - \nabla_P) F(\cdot)}{F(\cdot)} \Rightarrow 0 \quad \text{at } |\rho| \leq a, \quad (11)$$

where $\Omega = \rho/|\rho|$, and operators ∇_p and ∇_P do not touch the energy factor \mathcal{E} . Or, equivalently, - since region $|\rho| < a$ may be considered as forbidden after the hard-ball limit transition, -

$$\Omega \cdot (\nabla_p - \nabla_P) F(\rho = a\Omega) = 0, \quad (12)$$

again with ∇_p and ∇_P ignoring factor \mathcal{E} (which, of course, now turns to mere kinetic energy).

The Eq.12 thus must serve in place of Eq.3 in the role of boundary condition, in the $r - R = \rho$ -space, for probability density evolution equations. In other words, Eq.12 gives alternative to (3) non-conventional probability-theoretical representation of hard-ball collision rules.

B. Discussion. The alternative probabilistic formulation of hard-ball collision rules directly forbids Boltzmann's molecular chaos

1. One could see that just suggested unusual boundary condition (12) is logically implied by very simple and physically meaningful mathematical reasonings, in contrast to the traditional condition (3) which was merely postulated somewhere as naive literal reflection of mechanical relations (1)-(2).

The surface appearances of usual and alternative conditions also are quite different. Nevertheless, there is no qualitative disagreement between their mathematical contents. Indeed, notice, first, that factor \mathcal{E} in the DF $F(t, \dots \mathcal{E}, \rho, P, p \dots)$ in (12), - $\mathcal{E} = P^2/2M + p^2/2m$ after the hard-ball limit, - is invariant in respect to changing u to $u^* = u - 2\Omega(\Omega \cdot u)$, in accordance with (1)-(2). Second, if we represent the same DF through variables $P + p$ and $u = v - V = p/m - P/M$ instead of P and p , then condition (12) says that

$$\Omega \cdot \nabla_u F(t, \dots \mathcal{E}, \rho = a\Omega, P + p, u \dots) = 0 \quad (13)$$

at fixed \mathcal{E} . Hence, $F(\rho = a\Omega)$ has no dependence on normal component of relative velocity, $\Omega \cdot u$, at all.

As the consequence, obviously, summary DF's dependence on u satisfies $F(\rho = a\Omega, u) = F(\rho = a\Omega, u^*)$, that is our condition (12) contains conventional condition (3).

2. But the opposite statement generally is wrong. Therefore, our condition is more restrictive and may forbid somewhat allowed by the conventional one.

Anyway it is easy to make sure that in general the Boltzmann's "molecular chaos", that is pair DF's factorization for particles entering a collision (at $\rho \rightarrow a\Omega$, $\Omega \cdot u < 0$), certainly is forbidden. Indeed, according to the above derivation of our boundary condition (12), most general factorized DF can be expressed by

$$F(|\rho| = a) = e^{-\beta\mathcal{E}} A(R, P) B(R + a\Omega, p) ,$$

with some coefficient β , and \mathcal{E} not subject to the differentiation operators in Eqs.12-13 (thus acting onto product AB only). Then Eq.12 requires

$$\Omega \cdot \nabla_P \ln A(R, P) - \Omega \cdot \nabla_p \ln B(R + a\Omega, p) = 0$$

at any Ω . This is possible only when $A \propto \exp(c \cdot P)$ and $B \propto \exp(c \cdot p)$ with one and the same constant vector c and (omitted) proportionality coefficients depending respectively on R and r only.

Hence, the factorization is compatible with Eq.12 in the only case when momenta distribution is thermally equilibrium Maxwellian one (may be shifted in velocity space by c/β), i.e. when collisions make no effect at all.

3. Thus, interestingly, in the framework of our probability-theoretical representation of hard-ball collision rules, any particles taking part in mutual collision (at least factually resultant one) possess significant mutual statistical correlations. Moreover, these correlations nearly equally cover both post-collision ($\Omega \cdot u > 0$) and pre-collision ($\Omega \cdot u < 0$) configurations.

One can say that intervention of particles in same collision is sufficient cause for statistical inter-correlations between them. Characteristic "mathematical mechanisms" of creation of these correlations and their physical meaning were pointed out already in [3] and then many times discussed in other works [5].

Our present consideration newly shows how collisions-induced inter-particle correlations can manifest themselves even at level of separate collision event and single evolution equation. But, of course, in order to investigate conjugated statistics of actual random series of collision events, we need in full infinite BBGKY hierarchy.

IV. HARD-BALL BROWNIAN PARTICLE IN IDEAL GAS

First, let us recollect general case of smooth interaction potential.

A. BBGKY hierarchy for a smooth interaction potential

1. The BBGKY hierarchy, which describes "molecular Brownian particle" (BP) interacting with atoms of ideal gas, can be written as

$$\dot{F}_k = -V \cdot \nabla_R F_k - \sum_{j=1}^k \hat{L}_j F_k - n \nabla_P \int_{k+1} \Phi'(\rho_{k+1}) F_{k+1} \quad (14)$$

Here $k = 0, 1, \dots$ is number of gas atoms under simultaneous attention along with BP; F_k is corresponding $(k+1)$ -particle DF; \hat{L}_j is Liouville operator describing motion of j -numbered atom (atoms) and its (their) interaction with BP,

$$\hat{L}_j = -u_j \cdot \nabla_{\rho_j} + \Phi'(\rho_j) \cdot [\nabla_{p_j} - \nabla_P] ; \quad (15)$$

$\rho_j = r_j - R$, $u_j = v_j - V$, $v_j = p_j/m$, $V = P/M$; $\int_s \dots = \int \dots d\rho_s dp_s$, and n is mean gas density.

We are interested first of all in BP's random walk in thermodynamically equilibrium gas. Therefore, initial conditions to Eqs.14 will be

$$F_k|_{t=0} = \delta(R) G_M(P) \prod_{j=1}^k g(x_j) , \quad (16)$$

with notations $x = \{\rho, p\}$,

$$g(x) = E(\rho) G_m(p) ,$$

and

$$E(\rho) = \exp[-\Phi(\rho)/T] ,$$

$$G_m(p) = (2\pi Tm)^{-3/2} \exp(-p^2/2Tm)$$

(thus $G_m(\mathbf{p})$ denoting Maxwell momentum distribution of a particle with mass m).

Clearly, the corresponding DFs describe BP which at $t < 0$ was fixed near the coordinate origin, being surrounded by equilibrium gas, but at $t = 0$ becomes released. The release destroys statistical equilibrium (detailed balance) between BP and gas and initiates transition of the system to new equilibrium (new detailed balance) where BP's position will be fully uncertain. This process creates specifically non-equilibrium many-particle statistical correlations between BP and atoms. Full hierarchy of these correlations serves as "book-keeping report" accumulating information about *a posteriori* probabilities (actual statistical weights) of various BP's collision patterns and resulting trajectories.

To solve Eqs.14, we have also to take into account the trivial boundary conditions for DFs at infinity: $F_k \rightarrow$

$F_{k-1} G_m(\mathbf{p}_s)$ at $\rho_s \rightarrow \infty$, where $1 \leq s \leq k$ and F_{k-1} does not include ρ_s and p_s .

2. It may be useful to recollect method of generating functionals (GF) of DFs, - for the first time introduced by Bogolyubov in [8], - and exploit so-called “dynamical virial relations” (DVR) for the first time previewed in [13] and then substantiated and investigated in [14–18, 20, 21, 23].

Here, let us introduce GF by

$$\mathcal{F}\{t, R, V, \psi; n\} = F_0 + \sum_{s=1}^{\infty} \frac{1}{s!} \int_1 \dots \int_s F_s \prod_{j=1}^s \psi(x_j) \quad (17)$$

with formally arbitrary probe function $\psi(x)$. This GF obeys evolution equation

$$\dot{\mathcal{F}} = -V \cdot \nabla_R \mathcal{F} + \int_x [n + \psi(x)] \times \quad (18)$$

$$\times [(V - v) \cdot \nabla_\rho + \Phi'(\rho) \cdot (\nabla_p - \nabla_P)] \frac{\delta \mathcal{F}}{\delta \psi(x)},$$

which is equivalent to the whole hierarchy (14), with initial condition

$$\mathcal{F}(t=0) = \delta(R) G_M(P) \exp \int_x g(x) \psi(x), \quad (19)$$

equivalent to all (16).

What is for the DVR, for our particular system “BP in ideal gas” under initial conditions (16) we can express them e.g. in the form pointed out in [23],

$$\frac{\partial F_s}{\partial n} = \int_{s+1} [F_{s+1} - g(x_{s+1}) F_s] \quad (20)$$

Or, equivalently, in terms of the GF,

$$\frac{\partial \mathcal{F}}{\partial n} = \int_x \left[\frac{\delta}{\delta \psi(x)} - g(x) \right] \mathcal{F} \quad (21)$$

Notice that these DVR are valid also for arbitrary non-equilibrium initial gas states represented by any reasonable choice of the function $g(x)$ different from the above concretized one.

B. Conventional BBGKY hierarchy for hard-ball interaction

Following postulates of the conventional mathematical theory [1, 2], in case of hard-ball BP-atom interaction the BBGKY Eqs.14 should be replaced by

$$\dot{F}_k = -V \cdot \nabla_R F_k + \sum_{j=1}^k (V - v_j) \cdot \nabla_{\rho_j} F_k + \quad (22)$$

$$+ na^2 \oint \int dp_{k+1} (\Omega \cdot (v_{k+1} - V)) \times$$

$$\times F_{k+1}(\rho_{k+1} = a\Omega),$$

where $\oint \dots = \int \dots d\Omega$, and $|\rho_j| > a$. These equations must be supplied by boundary conditions like (3),

$$F_k(\rho_j = a\Omega_j, V, v_j) = F_k(\rho_j = a\Omega_j, V^*, v_j^*) \quad (23)$$

or, in terms of variables $v_j - V \equiv u_j$ and $P + p_j$, in view of the conservation $P + p_j = P^* + p_j^*$,

$$F_k(\rho_j = a\Omega_j, u_j) = F_k(\rho_j = a\Omega_j, u_j^*), \quad (24)$$

where $j = 1 \dots k$ and $|\Omega_j| = 1$.

At that, initial conditions corresponding to (16) are

$$F_k|_{t=0} = \delta(R) G_M(P) \prod_{j=1}^k G_m(p_j), \quad (25)$$

while the conditions (of weakening of correlations) at infinity are $F_k \rightarrow G_m(p_j) F_{k-1}$ at $\rho_j \rightarrow \infty$, with F_{k-1} independent on ρ_j and p_j .

C. Alternative BBGKY hierarchy for the hard-ball limit

Our above consideration prompts that before performing the hard-ball limit (8) in Eqs.14 it is necessary to extract from the DFs the ubiquitous thermodynamical factors and write

$$F_k = \exp(-\mathcal{E}_k/T) Q_k = \quad (26)$$

$$= \{ G_M(P) \prod_{j=1}^k E(\rho_j) G_m(p_j) \} \times Q_k,$$

where \mathcal{E}_k is energy of “BP plus k atoms”. Such defined functions Q_k just represent the mentioned perturbations of detailed balance and related non-equilibrium statistical correlations.

Then, we must take into account that, naturally, characteristic energies (per one particle), conjugated with these perturbations and correlations, remain finite under the limit (8). Therefore, all the functions Q_k (with $k > 0$) remain continuous smooth functions of the distances ρ_j , in the sense that formally all these functions stay continuously extendable into regions $|\rho_j| < a$.

In such way we come to the hard-ball limit scheme formulated in Section III. Applying its collision boundary condition, Eq.12, in Eqs.14, together with Eqs.26, after elementary manipulations and reasonings it is not hard to arrive to equations

$$\begin{aligned} \dot{Q}_k = & -V \cdot \nabla_R Q_k + \sum_{j=1}^k (V - v_j) \cdot \nabla_{\rho_j} Q_k + \\ & + na^2 \oint \int dp_{k+1} (\Omega \cdot (v_{k+1} - V)) \times \\ & \times G_m(p_{k+1}) Q_{k+1}(\rho_{k+1} = a\Omega) , \end{aligned} \quad (27)$$

again with $\oint \dots = \int \dots d\Omega$, and $|\rho_j| \geq a$, but now to be supplied by boundary conditions very visually different from (23). Namely,

$$\Omega_j \cdot (\nabla_{\rho_j} - \nabla_P) Q_k(\rho_j = a\Omega_j) = 0 , \quad (28)$$

where $j = 1 \dots k$ and $|\Omega_j| = 1$.

This is our hard-ball limit case of the BBGKY hierarchy for “BP in ideal gas”. Clearly, the mentioned initial conditions to it now look as

$$Q_k|_{t=0} = \delta(R) , \quad (29)$$

while the conditions (of weakening of correlations) at infinity now state that $Q_k \rightarrow Q_{k-1}$ at $\rho_j \rightarrow \infty$, with Q_{k-1} free of ρ_j and p_j .

D. Hard-ball BBGKY hierarchy in terms of cumulant (correlation) distribution functions

1. Just presented equations (27) by themselves have no essential difference from equations (22) of conventional theory. Indeed, the latter turn to the former after replacement

$$F_k = \{ G_M(P) \prod_{j=1}^k G_m(p_j) \} \times Q_k , \quad (30)$$

so that the only actual difference between alternative and conventional formalisms is in their collision (contact) boundary conditions. Namely, our ones are given by Eqs.28, while conventional, Eqs.23, - when considered in terms of Q_k from (30), - appear from Eqs.23 by mere inserting Q_k in place of F_k .

Hence, the concept of *cumulant*, or *correlation*, functions (CF) [6, 25] directly transmits to our formalism. Designating them by C_k , as in [6], and introducing like there, but now through Q_k ’s instead of F_k ’s, we have to write

$$\begin{aligned} Q_0(t, R, P) &= C_0(t, R, P) , \\ Q_1(t, R, P, x_1) &= C_0(t, R, P) + C_1(t, R, P, x_1) , \\ Q_2(t, R, P, x_1, x_2) &= C_0(t, R, P) + \\ &+ C_1(t, R, P, x_1) + C_1(t, R, P, x_2) + \\ &+ C_2(t, R, P, x_1, x_2) , \end{aligned} \quad (31)$$

and so on.

Clearly, advantage of such defined “cumulant functions” (CF) C_k is that they vanish at infinity: $C_k \rightarrow 0$ at $\rho_j \rightarrow \infty$. Therefore one can integrate them over relative distances. This means that C_k represent most connected, or irreducible, $(k+1)$ -particle correlations. Correspondingly, initial conditions (29) in their terms look maximally simple:

$$C_k|_{t=0} = \delta_{k0} \delta(R) \quad (32)$$

What is for evolution equations fore the CFs, in case of hard-ball interaction they look exactly as Eqs.27 minus symbol Q ’s replacement by C :

$$\begin{aligned} \dot{C}_k = & -V \cdot \nabla_R C_k + \sum_{j=1}^k (V - v_j) \cdot \nabla_{\rho_j} C_k + \\ & + na^2 \oint \int dp_{k+1} (\Omega \cdot (v_{k+1} - V)) \times \\ & \times G_m(p_{k+1}) C_{k+1}(\rho_{k+1} = a\Omega) \end{aligned} \quad (33)$$

However, the collision boundary conditions for these equations essentially differ from (28) or (23) since now connect CFs with two neighboring numbers. Namely, in conventional formalism [6]

$$\begin{aligned} C_k(\rho_j = a\Omega_j, P, p_j) + C_{k-1}(P) = \\ = C_k(\rho_j = a\Omega_j, P^*, p_j^*) + C_{k-1}(P^*) \end{aligned} \quad (34)$$

while in alternative formalism

$$\Omega_j \cdot (\nabla_{\rho_j} - \nabla_P) [C_k(\rho_j = a\Omega_j, P, p_j) + C_{k-1}(P)] = 0 \quad (35)$$

These formulas follow from the above CFs definition (31) as applied to (23) or (28). In both them C_{k-1} does not concern j -th atom, and we omitted all arguments not concerned by a collision under consideration.

2. In the hard-ball limit the DVR (20) yield

$$\begin{aligned} \frac{\partial Q_s}{\partial n} &= \int_{\rho: |\rho| > a} \int_p G_m(p) [Q_{s+1} - Q_s] , \\ \frac{\partial C_s}{\partial n} &= \int_{\rho: |\rho| > a} \int_p G_m(p) C_{s+1} , \end{aligned} \quad (36)$$

with $\rho = \rho_{s+1}$ and $p = p_{s+1}$.

Importantly, these relations hold regardless of choice of collision boundary conditions. The latter circumstance is due to fact that generally DVR are insensitive to character of interactions. This is because DVR are expression of general kinematic properties of (infinitely) many-particle dynamical systems, first of all, the phase volume conservation there (expressed also by the “Liouville theorem” and “fluctuation-dissipation relations” [22]).

3. One can see that irreducible correlations of given order arise either from lower-order correlations, via the collision boundary conditions, or from higher-order correlations, via the “collision integrals”. Of course, at initial stage of evolution the first of these two opposite flows of correlations is dominating. But later, at kinetic stage, their approximate balance may be expected. It then establishes some spatial bounds correlated clusters, so that C_k ’s extension in ρ_j -spaces is not growing unboundedly with time.

According to theorem, or “lemma”, proved in [14, 15, 17], such behavior of inter-particle correlations means presence of time-scaleless $1/f$ -type fluctuations of BP’s diffusivity (mobility [9, 10]). A simple substantiation of this statement, basing on simplest of the DVR, was demonstrated in [22, 23].

E. Hard-ball limit of generating functional equations and dynamical virial relations

In terms of generating functional (GF) introduced by

$$\mathcal{Q}\{t, R, V, \psi; n\} = Q_0 + \sum_{s=1}^{\infty} \frac{1}{s!} \int_1 \dots \int_s Q_s \prod_{j=1}^s \psi(x_j), \quad (37)$$

our equations (27) and conditions (28) can be unified into

$$\begin{aligned} \dot{Q} = & -V \cdot \nabla_R Q + \\ & + \int_x [n G_m(p) \theta(|\rho| - a) + \psi(x)] \times \\ & \times ((V - v) \cdot \nabla_\rho) \frac{\delta Q}{\delta \psi(x)}, \end{aligned} \quad (38)$$

with $\theta(\cdot)$ being the Heaviside step function, and

$$\oint \int_p \psi(a\Omega, p) (\Omega \cdot (\nabla_p - \nabla_P)) \frac{\delta Q}{\delta \psi(a\Omega, p)} = 0 \quad (39)$$

At that, generating DVR (21) transforms to

$$\frac{\partial Q}{\partial n} = \int_{|\rho| > a} \int_p G_m(p) \left[\frac{\delta}{\delta \psi(x)} - 1 \right] Q \quad (40)$$

It is easy deducable directly from Eq.38.

To rewrite these generating relation in the CF’s language, one has to notice that

$$\mathcal{Q}\{t, R, V, \psi; n\} = e^{\int \psi(x) dx} \mathcal{C}\{t, R, V, \psi; n\}, \quad (41)$$

where \mathcal{C} is CF’s GF introduced similarly to (37).

V. COMPARISON BETWEEN STANDARD AND ALTERNATIVE TREATMENTS OF (HARD-BALL) STATISTICAL MECHANICS

Although evolution equations in the two approaches are coinciding, their unambiguous solution is impossible without definite collision boundary conditions. But right there the coincidence ends.

A. Why conventional collision boundary conditions seem unsatisfactory

For the first look, our boundary conditions for probability densities at inter-particle contact surfaces, - (12), (28), (35) and (39), - are rather complicated and non-transparent in comparison with standard conditions, - (3), (23) and (34). Therefore, it is important to emphasize once more their advantages.

In both the Eqs.22 and Eqs.27 the “extra particle” integral terms, - which eventually must play roles of “collision integrals”, - are functionals of edge boundary values of DFs at $|\rho_{k+1}| = a$. Hence, we have all rights, - moreover, are forced, - to be interested in such edge values of DFs anywhere else besides the integral terms. This then requires to consider many-particle configurations where simultaneously $|\rho_{k+1}| \rightarrow a$ and $|\rho_j| \rightarrow a$, and so on. Consequently, in general, we need in some boundary conditions for situations when simultaneously two or several atoms are in contact with BP or in its arbitrary close vicinity.

That is non-trivial question. Unfortunately, in the context of conventional theory there is no ready answer to it or a recipe for getting such answer. In any case, one can verify that literal parallel application of two or several samples of the condition (23) can not be a suitable rule for configurations with two or several $|\rho_j| \rightarrow a$ at once, since it is incompatible with conservation of both total momentum and total kinetic energy of involved particles.

This fact once again demonstrates that the conventional theory is formally incomplete. Therefore, there we are enforced to treat the mentioned configurations as three- or many-particle processes constituted by two or more almost simultaneous pair collisions. Then one meets extremely complicated task of geometric and kinematic classification of infinite variety of such processes. By such reasons, strictly speaking, the conventional theory seems still rather bad developed.

B. On problems of probabilistic description of infinitely-many-particle systems

1. In this theory (see e.g. [1, 2] and reference therein) just underlined problems traditionally were avoided, - taking in mind the Boltzmann-Grad limit (BGL), - by means of artificial exclusion of “unpleasant” configurations leading to the mentioned many-particle events, i.e. to sticking together, or “glued”, pair collisions. This is achieved by means of a proper selection of initial conditions under term-by-term consideration of BGL of formal iteration series for BBGKY hierarchy. Such the “art” is motivated by small statistical weight (zero in the BGL) of the unpleasant configurations.

However, this is bad idea, because any equation of the BBGKY hierarchy and any DF there represents 1, 2, 3 ... particles moving among infinitely many other particles constituting full system, while any term of the iteration series says something about motion of namely 1, 2, 3 ... particles without others. At that, actual “probabilities” of 2, 3, 4 ... -particle configurations and events in real infinite system hardly are proportional to statistical weights defined for similar configurations and events in a group of fixed finite number of particles.

2. Thus, one should remember that actual statistical effects of collisions are determined by not *a priori* statistical weights or expectations but *a posteriori* conditional probability densities which reflect both current surroundings of colliding particles and pre-history of the system’s evolution. For instance, in Eqs.27, by means of factors

$$Q'_{k+1}(\Omega, P, p_{k+1} | t, R, x_1 \dots x_k) = Q_{k+1}(\rho_{k+1} = a\Omega) / Q_k, \quad (42)$$

which, at $\Omega \cdot u_{k+1} < 0$, visually modify “probability of collision” or “differential cross-section of collision”, - between BP and “outer” $(k+1)$ -th atom, - in comparison with what would take place if we considered two isolated particles only in a pre-collision state.

In reality, the colliding particles acquire some *conditional* correlation, - in the sense of the probability theory, - conditioned by an information about k other gas atoms from BP’s surroundings. The factor (42), representing such correlations, more or less differs from unit, $Q'_{k+1}(\cdot) \neq 1$, in particular, if presented information indicates possibility of BP’s interaction with some of that k atoms in the past. For instance, when the “outer” $(k+1)$ -th atom in fact could not arrive closely to BP (to position with $|\rho_{k+1}| \rightarrow a$) directly “from infinity” (its start position at $t = 0$) since continuation of its straight-line trajectory into the past intersects preceding BP’s trajectory as bent by past BP’s collision with some of other given k atoms.

In the latter case we meet situation of “forbidden” (or “impossible” or “virtual”) repeated collision, for which we may then suppose that $Q'_{k+1}(\cdot) < 1$. Another particular variant of “unpleasant” configuration is when it

indicates seemingly allowed “repeated collisions”. Both these examples can be illustrated by figure in [6].

3. More complicated cases combine hints of both forbidden and allowed “repeated collisions”. Of course, relative probability of such events vanishes under the BGL (when $a^3 n \rightarrow 0$ while $a^2 n = \text{const}$) if they are considered from viewpoint of arbitrary initial conditions. However, if being considered from viewpoint of already happened configurations with $|\rho_j| \sim a$, they acquire conditional probabilities non-vanishing even in BGL. More precisely, if all arguments ρ_j ($j = 1 \dots k$) in $Q'_{k+1}(\Omega, P, p_{k+1} | t, R, x_1 \dots x_k)$ are kept comparable with a , then, under proper p_j ($j = 1 \dots k$), a portion of p_{k+1} ’s values (weighted with $G_m(p_{k+1})$), responding to earlier happened interaction between the “outer” atom and BP, stays comparable with unit (tend to non-zero constant), so that $Q'_{k+1} \neq 1$, in spite of BGL. Hence, “unpleasant” configurations may play important, if not decisive, role in true solution to Eqs.27 (see [21, 23] and references therein).

4. Another very important thing is that a part of the mentioned “earlier happened” BP-atom interactions is delegated by the *seed* (equilibrium) BP-atoms correlations represented by function $g(x) = G_m(p) \exp[-\Phi(p)/T]$, - or $g(x) \rightarrow G_m(p) \theta(|rho| - a)$ for the hard-ball limit, - in the initial conditions Eq.16. Therefore, formal expression seemingly describing a repeated collision in essence may be description of two stages of one and the same BP-atom collision but statistically influenced by both the seed initial correlations and later generated non-equilibrium correlations due to BP’s interaction with the rest of gas.

The diagram on figure in [6] applies also to this simple case if we interpret inscriptions C_1^{out} and C_1^{in} there as symbols of “output from initial equilibrium correlation” and “input to non-equilibrium correlation”, respectively, while C_2 as symbol of “influence by the rest of gas” (which just causes a difference $Q'_1(\cdot) \neq 1$).

The latter then is not simultaneous intervention of a third particle (atom) but instead interference of previous BP’s collisions which altogether transform “probability” or “(differential) cross-section” of the current collision into random quantity without a priori known average value. More precisely, with a value whose true prediction needs in honest solution of the BBGKY hierarchy (e.g. in terms of the factors $Q'_{k+1}(\cdot)$).

Such kind of interference of “the rest of gas” in particular collision event surely survives under BGL along with corresponding statistical correlations caught in the CFs and Q' ’s.

Unfortunately, these rather fine aspects insensibly disappear in the framework of conventional theory, because it operates with initial correlations as if $g(x) \rightarrow G_m(p)$. As the consequence, it incorrectly reproduces action of operators \hat{L}_j onto initial DFs $F_k(t=0)$.

However, one can avoid such defects if rearranging BGL and hard-ball limit. Other way to correct the the-

ory may be to use so-called “pseudo-Liouville representation” of hard-ball interaction [1, 2] which allows us to unify both the hard-ball BBGKY equations and collision boundary conditions (CBC) (23) into single generating functional (GF) evolution equation similar to Eq.gfe.

Therefore it is useful to discuss it, first of all, for smooth interactions, in order to demonstrate character of statistical connections between next BP-atom collision and history of earlier BP’s interaction with the rest of gas.

C. Exact pseudo-kinetic generating-functional formulation of BBGKY hierarchy and crash of Boltzmann’s kinetics

1. Let us introduce functional (differential) operator

$$\begin{aligned}\widehat{\mathcal{L}} &= \widehat{\mathcal{L}}\{V, \psi, \nabla_P, \delta/\delta\psi\} = \\ &= \int_x [n + \psi(x)] \widehat{L}_x(V, \nabla_P) \frac{\delta}{\delta\psi(x)},\end{aligned}\quad (43)$$

where \widehat{L}_x is abstraction of operators \widehat{L}_j ,

$$\begin{aligned}\widehat{L}_x &= \widehat{L}_x(V, \nabla_P) = \\ &= (V - v) \cdot \nabla_\rho + \Phi'(\rho) \cdot (\nabla_p - \nabla_P)\end{aligned}\quad (44)$$

Besides, it is comfortable to introduce operators

$$\begin{aligned}\widehat{\mathcal{L}}' &= e^{-\int g(x) \psi(x) dx} \widehat{\mathcal{L}} e^{\int g(x) \psi(x) dx} = \\ &= \int_x [n + \psi(x)] \widehat{L}_x(V, \nabla_P) \left[\frac{\delta}{\delta\psi(x)} + g(x) \right], \\ \widehat{\mathcal{L}}_R &= -V \cdot \nabla_R + \widehat{\mathcal{L}}, \quad \widehat{\mathcal{L}}'_R = -V \cdot \nabla_R + \widehat{\mathcal{L}}'\end{aligned}\quad (45)$$

In parallel, recall definition of the correlation, or cumulant, functions (CF) for general (not hard-ball) BP-atom interaction potential,

$$\begin{aligned}F_0(t, R, P) &= C_0(t, R, P), \\ F_1(t, R, P, x_1) &= C_0(t, R, P) g(x_1) + C_1(t, R, P, x_1), \\ F_2(t, R, P, x_1, x_2) &= C_0(t, R, P) g(x_1) g(x_2) + \\ &+ C_1(t, R, P, x_1) g(x_2) + C_1(t, R, P, x_2) g(x_1) + \\ &+ C_2(t, R, P, x_1, x_2),\end{aligned}\quad (46)$$

and so on, and their generating functional (GF),

$$\mathcal{F}\{t, R, V, \psi; n\} = e^{\int_x g(x) \psi(x)} \mathcal{C}\{t, R, V, \psi; n\} \quad (47)$$

Then the functional evolution equation Eq.18 reads shortly as

$$\partial_t \mathcal{F} = -V \cdot \nabla_R \mathcal{F} + \widehat{\mathcal{L}} \mathcal{F} = \widehat{\mathcal{L}}_R \mathcal{F}, \quad (48)$$

while equivalent equation for CF’s GF as

$$\partial_t \mathcal{C} = -V \cdot \nabla_R \mathcal{C} + \widehat{\mathcal{L}}' \mathcal{C} = \widehat{\mathcal{L}}'_R \mathcal{C} \quad (49)$$

with initial condition

$$\mathcal{C}(t=0) = \delta(R) G_M(P) \quad (50)$$

equivalent to all (16) and independent on the probe-function argument $\psi(x)$.

2. Next, let us rewrite Eq.48 in the form

$$\partial_t \mathcal{F} = -V \cdot \nabla_R \mathcal{F} + \int_x [n + \psi(x)] \widehat{L}_x(V, \nabla_P) \mathcal{F}_x \quad (51)$$

where we introduced derivative

$$\mathcal{F}_x = \frac{\delta \mathcal{F}}{\delta \psi(x)},$$

and supplement Eq.51 with equation for \mathcal{F}_x directly following from Eq.48,

$$\partial_t \mathcal{F}_x = [-V \cdot \nabla_R + \widehat{L}_x + \widehat{\mathcal{L}}] \mathcal{F}_x, \quad (52)$$

with obvious initial condition

$$\mathcal{F}_x(t=0) = g(x) \mathcal{F}(t=0)$$

Combining all these formulas, it is easy to transform Eqs.48 and 49 to

$$\begin{aligned}\partial_t \mathcal{F} &= -V \cdot \nabla_R \mathcal{F} + \widehat{\mathcal{K}}(t) \mathcal{F}, \\ \partial_t \mathcal{C} &= -V \cdot \nabla_R \mathcal{C} + \widehat{\mathcal{K}}'(t) \mathcal{C},\end{aligned}\quad (53)$$

with new operators

$$\begin{aligned}\widehat{\mathcal{K}}(t) &= \int_x [n + \psi(x)] \widehat{L}_x \times \\ &\times \exp[(\widehat{L}_x + \widehat{\mathcal{L}}_R) t] g(x) \exp[-\widehat{\mathcal{L}}_R t], \\ \widehat{\mathcal{K}}'(t) &= \int_x [n + \psi(x)] \widehat{L}_x \times \\ &\times \exp[(\widehat{L}_x + \widehat{\mathcal{L}}'_R) t] g(x) \exp[-\widehat{\mathcal{L}}'_R t]\end{aligned}\quad (54)$$

The latter un turn can be transformed like

$$\begin{aligned}\widehat{\mathcal{K}}'(t) &= \int_x [n + \psi(x)] \widehat{L}_x \{ g(x) + \int_0^t d\tau \partial_\tau \times, \\ &\times \exp[(\widehat{L}_x + \widehat{\mathcal{L}}'_R) \tau] g(x) \exp[-\widehat{\mathcal{L}}'_R \tau] \} = \\ &= [\int_x \psi(x) \widehat{L}_x g(x)] + \\ &+ \int_x [n + \psi(x)] \widehat{L}_x \int_0^t d\tau \times \\ &\times \exp[(\widehat{L}_x + \widehat{\mathcal{L}}'_R) \tau] \widehat{L}_x g(x) \exp[-\widehat{\mathcal{L}}'_R \tau]\end{aligned}\quad (55)$$

or, equivalently,

$$\begin{aligned} \hat{\mathcal{K}}'(t) &= \int_x \psi(x) \hat{L}_x \times \\ &\times \exp[(\hat{L}_x + \hat{\mathcal{L}}'_R)t] g(x) \exp[-\hat{\mathcal{L}}'_R t] + \\ &+ n \int_x \hat{L}_x \int_0^t d\tau \exp[(\hat{L}_x + \hat{\mathcal{L}}'_R)\tau] \hat{L}_x g(x) \exp[-\hat{\mathcal{L}}'_R \tau] \end{aligned} \quad (56)$$

Here expression $\hat{L}_x g(x)$ in fact acts as operator

$$\hat{L}_x g(x) = (\nabla_\rho g(x)) \cdot [V + T \nabla_P],$$

and we took into account that, obviously,

$$\int_x \hat{L}_x g(x) = 0$$

3. Eventually we are mainly interested not in the CFs themselves or their GF but in the BP's distribution function (DF)

$$F_0(t, R, P) = \mathcal{F}\{\psi = 0\} = \mathcal{C}\{\psi = 0\}$$

From its viewpoint, the argument $\psi(x)$ serves as “thermostat random field variable” responsible for both “stochastic agitation” of BP's velocity and its “irreversible relaxation”, while the operation $\psi(x) \rightarrow 0$, - if performed after all calculations, - as ensemble averaging over thermostat. In this sense, two terms in Eqs.55 and 56 can be interpreted as “random (Langevin) source” and “kinetic operator”, although, obviously, such separation is not unambiguous.

Advantage of representation Eqs.53-56, - in comparison with its origin, i.e. evolution equation Eq.49, - is in that it makes explicit visual step from instant interparticle potential interaction to time-distributed collision events. This becomes quite clear if we eliminate action of the thermostat in expression (55) or (56) by removing $\psi(x)$ and $\hat{\mathcal{L}}$ or $\hat{\mathcal{L}}'$, so that exact Eq.53 simplifies approximately to

$$\begin{aligned} \hat{\mathcal{K}}(t) &\approx \hat{\mathcal{K}}'(t) \approx n \int_x \hat{L}_x \int_0^t d\tau \times \\ &\times \exp[(\hat{L}_x - V \cdot \nabla_R) \tau] \hat{L}_x g(x) \exp[V \cdot \nabla_R \tau] \approx \\ &\approx \frac{n}{T} \int_0^\infty d\tau \nabla_P \cdot \int_x \Phi'(\rho) \times \\ &\times \exp[\hat{L}_x \tau] g(x) \Phi'(\rho) \cdot (V + T \nabla_P) \equiv \hat{B} \end{aligned} \quad (57)$$

This operator \hat{B} is nothing but usual (although non-standardly written [16]) Boltzmann-Lorentz kinetic operator (BLO) describing BP-gas interaction in Boltzmannian kinetics.

4. The last simplification in Eq.57 neglects contribution of BP's displacements during collisions to total BP's

pah, which is reasonable for rarefied gas, all the more in Boltzmann-Grad limit (BGL).

However, approximation (57) on the whole neglects also much more significant matter, namely, “geometrical contest” of particles (atoms) in collisions wit given one (BP). It means merely that realization of any particular current collision is conditioned by all before happened collisions: if one of them had different impact parameter or had no place at all, then all later collisions also would have different impact parameter values, moreover, almost surely would be prevented at all. Therefore, factually, differential cross-section of current collision is very complicated function of its pre-history.

In other words, differential cross-section of current collision is highly irregular function of initial state of the system,. Moreover, so much irregular that we certainly can not speak about its time-average value and, hence, its *a priori* value. Indeed, number of initial gas parameters, which potentially may influence on BP's motion during time t , grows with time roughly $\propto n(u_0 t)^3$ (with u_0 denoting characteristic thermal velocity) while number of BP's trajectory parameters $\propto t/\tau_0 \sim u_0 t/\lambda \sim n a^2 u_0 t$ (with τ_0 being characteristic BP's free path time), that is $\sim (u_0 t/a)^2$ times smaller. Clearly, so relatively small number of collision events in no way is sufficient for their time averaging in respect to all of their potential reasons.

Consequently, there are no statistical grounds to assume *a priori* definite (differential) cross-section for them. Moreover, the deeper we go to BGL, the lesser are such grounds (see also e.g. [12, 17, 22]. for similar argumentation).

5. The aforesaid is fully ignored in the “Boltzmannian kinetics” approximation (57). It can be rewritten, under same simplification (rejecting BP's shift during collision), in the form

$$\hat{\mathcal{K}}'(t) \approx n \int_x \hat{L}_x \exp[\hat{L}_x t] g(x), \quad (58)$$

which visually claims uniform distribution of collision's impact parameter (two-dimensional ρ 's projection onto plane $\perp u$). To compare this with the exact Eq.54, the latter can be expressed by

$$\begin{aligned} \hat{\mathcal{K}}'(t) &= \int_x [n + \psi(x)] \hat{L}_x \times \\ &\times \exp[\hat{L}_x t] \hat{\sigma}_x\{t, \psi\} g(x), \quad (59) \\ \hat{\sigma}_x\{t, \psi\} &= \exp[-\hat{L}_x t] \exp[(\hat{L}_x + \hat{\mathcal{L}}'_R)t] \exp[-\hat{\mathcal{L}}'_R t] \end{aligned}$$

Here operator $\hat{\sigma}_x\{t, \psi\}$ (together with also important factor $n + \psi(x)$ in place of n on the left) represents now randomly non-uniform impact parameter distribution.

Evidently, it involves all the past evolution time, thus, potentially all atoms what might achieve BP after its start, and establishes some statistical connection of current collision to micro-state of the rest of gas and, hence, to all earlier collisions.

Let us show that such connection survives, moreover, remains substantial and practically important, under BGL.

6. For this purpose, we have to return from Eq.59 to equivalent Eq.55 since it clearly distinguishes total evolution time t and much smaller “inner time” of collision τ . Then, for transparent transition to BGL there, make scale transformations

$$n \Rightarrow \frac{n}{\xi^2}, \quad \Phi(\rho) \Rightarrow \Phi\left(\frac{\rho}{\xi}\right), \quad (60)$$

where $\xi \rightarrow 0$, and simultaneously, in the integrals over $x = \{\rho, p\}$ and τ , make changes of integration variables and the “thermostat field” variable, as follow,

$$\rho \Rightarrow \xi \rho, \quad \psi(\xi \rho, p) \Rightarrow \frac{\psi(\rho, p)}{\xi^2}, \quad \tau \Rightarrow \xi \tau \quad (61)$$

The middle of these changes combines scale transformation, like that of the mean gas density in (60), and replacement $\psi(\xi \rho, p) \Rightarrow \psi(\rho, p)$. The latter should be applied, - inside $\hat{\mathcal{L}}$ and $\hat{\mathcal{L}}'$ or similar objects, - together with functional derivative transform

$$\frac{\delta}{\delta \psi(\xi \rho, p)} \Rightarrow \frac{\delta}{\xi^3 \delta \psi(\rho, p)} \quad (62)$$

This rule reflects invariance of “number-of-particles operator” in respect to our changes,

$$\begin{aligned} \int_x \psi(x) \frac{\delta}{\delta \psi(x)} &\equiv \int d^3 p \int d^3 \rho \psi(\rho, p) \frac{\delta}{\delta \psi(\rho, p)} = \\ &= \int d^3 p \int \xi^3 d^3 \rho \psi(\xi \rho, p) \frac{\delta}{\delta \psi(\xi \rho, p)} \end{aligned}$$

Taking all this into account, it is easy to verify that in the BGL, $\xi \rightarrow 0$, both the evolution operators $\hat{\mathcal{L}}$ (43) and $\hat{\mathcal{L}}'$ (45) are rescaled equally as

$$\hat{\mathcal{L}}, \hat{\mathcal{L}}' \Rightarrow \frac{\hat{\mathcal{L}}}{\xi} = \frac{1}{\xi} \int_x [n + \psi(x)] \hat{L}_x \frac{\delta}{\delta \psi(x)}, \quad (63)$$

while both the corresponding “pseudo-kinetic” operators (54) tend to one and the same limit,

$$\begin{aligned} \hat{\mathcal{K}}(t), \hat{\mathcal{K}}'(t) &\Rightarrow \hat{\mathcal{K}}_\infty = \int_x \psi(x) \hat{L}_x g(x) + \\ &+ \int_x [n + \psi(x)] \hat{L}_x \int_0^\infty d\tau \times \\ &\times \exp[(\hat{L}_x + \hat{\mathcal{L}})\tau] \hat{L}_x g(x) \exp[-\hat{\mathcal{L}}\tau] \end{aligned} \quad (64)$$

At that, according to above consideration,

$$F_0(t, R, P) \Rightarrow \left\langle e^{(-V \cdot \nabla_R + \hat{\mathcal{K}}_\infty)t} \right\rangle F_0(0, R, P) \quad (65)$$

with angle brackets meaning statistical averaging as defined by

$$\langle \dots \rangle = [\dots]_{\psi=0}$$

Of course, after transition to BGL, results of the averaging depend on the composite parameter $a^2 n = (\pi \lambda)^{-1}$ as the whole only.

In particular, on average the limit random “pseudo-kinetic” operator (64) coincides with the Boltzmann-Lorentz one from (57),

$$\langle \hat{\mathcal{K}}_\infty \rangle = \hat{B},$$

while for its variance Eq.64 formally yields

$$\begin{aligned} \langle \hat{\mathcal{K}}_\infty^2 \rangle - \langle \hat{\mathcal{K}}_\infty \rangle^2 &= n^2 \int_x \int_y \int_0^\infty d\tau \int_0^\infty d\tau' \times \\ &\times \hat{L}_x [e^{\hat{L}_x \tau} \hat{L}_y e^{(\hat{L}_x + \hat{L}_y)\tau'} \hat{L}_x e^{-\hat{L}_y(\tau + \tau')} - \\ &- e^{\hat{L}_x(\tau + \tau')} \hat{L}_x \hat{L}_y e^{-\hat{L}_y \tau'}] \hat{L}_y g(y) g(x), \end{aligned} \quad (66)$$

where, clearly, x and y are two different atom’s phase points (each pointing to momentum and relative distance). This expression, by its nature, represents just mutual interference of gas atoms in possibilities of their encounters with BP.

7. Thus, we have demonstrated that in general BGL produces a non-trivial theory principally and quantitatively different from Boltzmann’s kinetics.

At that, all the CFs possess also non-trivial non-zero limits, though they require special careful consideration since are singular functions with two “infinitely strongly” different spatial scales, a and λ .

It is useful to take in mind that corresponding inter-particle statistical correlations have no an “autonomous” physical meaning (“mechanism”) but, in essence, are originated by mere knowledge about past BP’s walk (path). In other words, about practically observed rate of system’s evolution to final statistical equilibrium where $\nabla_R F_0 \rightarrow 0$. Indeed, a greater value of BP’s path gives evidence of its faster diffusion and lesser rate (relative frequency) of its collisions, or smaller efficiency (effective cross-section) of collisions, - and vice versa, - which is just the source of BP-atoms correlations.

From formal viewpoint of BBGKY equations, inequality $\nabla_R F_0 \neq 0$ implies violation of equilibrium (Maxwellian) character of BP’s velocity distribution, which in turn inevitably induces various inter-particle correlations.

From physical viewpoint, the system (gas) forgives deviations of rate (relative frequency and efficiency) of BP’s collisions from its imaginary “mean value”. Therefore, each particular realization of BP’s life (trajectory) randomly acquires its own unique time-averaged collision

rate [3, 9–11, 22, 24]. Then all atoms somehow (actually or virtually) involved into BP's life become “guilty of” (correlated with) its unpredictable result.

D. Why alternative collision boundary conditions seem good

Advantage of our probability-theoretical formulation of the hard-ball collision rules, - i.e. conditions (12) and (28) or (35), - is that it creates no questions when being applied to configurations characterized by two or several $|\rho_j| \rightarrow a$ at once. The matter is that different conditions from a set (28) are freely compatible one with another, because all they are mutually commutative, in contrast to conventional conditions from (23).

Due to this fact, now we obviate the necessity of artificial division of many-particle configurations like three- or multi-particle collisions into almost simultaneous pair collisions. At the same time, we can consider arbitrary chains and graphs of more or less close pair collisions, being guaranteed for smooth unambiguous transition from them to “many-particle collisions”.

Thus, the related formalism, in contrast to conventional one, is logically complete and unambiguous. This is good stimulus for investigation of its principal consequences and practical utility. At present, we confine ourselves by its preliminary discussion only.

VI. PRINCIPAL PROPERTIES OF HARD-BALL BBGKY HIERARCHY AND EXPECTED SOLUTIONS TO IT

A. Possibility of continuation to the whole ρ -space

1. According to above derivation of our of hard-ball BBGKY hierarchy, Eqs.27, the functions Q_k , (with $k > 0$) there are such that can be continuously extended into (physically forbidden) regions $|\rho_j| < a$, for some or each of $1 \leq j \leq k$. In corresponding version of the theory, the collision boundary conditions (CBC) (28) must be replaced by ones which follow from Eq.11, that is

$$\Omega_j \cdot (\nabla_{p_j} - \nabla_P) Q_k(\cdot) = 0 \quad \text{at} \quad |\rho_j| \leq a \quad (67)$$

At that, besides, the Eqs.27 themselves must be modified too, since, - in view of Eq.10, - the limit expressions

$$\frac{\Phi'(\rho_j) \cdot (\nabla_{p_j} - \nabla_P) Q_k}{Q_k} \Rightarrow \gamma_k(\cdot)$$

may be thought having non-zero finite values, in spite of zero in Eq.11. Therefore, now we should write

$$\begin{aligned} \dot{Q}_k = & \gamma_k Q_k - V \cdot \nabla_R Q_k + \sum_{j=1}^k (V - v_j) \cdot \nabla_{\rho_j} Q_k + \\ & + na^2 \oint \int dp_{k+1} (\Omega \cdot (v_{k+1} - V)) \times \\ & \times G_m(p_{k+1}) Q_{k+1}(\rho_{k+1} = a\Omega) \end{aligned} \quad (68)$$

Here ρ_j take arbitrary values, and the “sources” $\gamma_k Q_k$ have appeared, which can differ from zero in the forbidden regions only ($\gamma_k(\cdot) \neq 0$ if and only if $|\rho_j| < a$ for at least one of $1 \leq j \leq k$) and must be chosen in such a way that all the conditions (67) are satisfied.

Possible advantage of this formalism, as compared with Eqs.27 plus 28, is obvious: it allows to represent all Q_k 's by evident iteration series free of CBC which now transform into integral equations for the sources.

2. In the conventional approach too there is possibility to go to the whole ρ -space (“without holes”) if introducing proper source terms. In particular, sources can be concentrated at boundaries of forbidden regions, i.e. at $|\rho_j| = a$. In such way one can include all the CBC (23) to sources and thus automatize their use.

The corresponding form of BBGKY equations was mentioned e.g. in [2] as “pseudo-Liouville”. In principle, it brings help for objective evaluation of contributions from specific “unpleasant” many-particle configurations and events, avoiding their artificial sorting out and thus preventing crucial losses of standard formalism [1, 2]. Such ability of “pseudo-Liouville” representation was demonstrated in [7].

B. Density of collisions drifts with centre-of-mass velocity

1. The integral terms in Eqs.27 (as well as in Eqs.14), - responsible for collisions with “outside” particles, - are determined by space-angle averaging in ρ -space and vector functions like

$$A_{kj} = \oint \Omega Q_k(\rho_j = a\Omega) \quad (69)$$

The same functions appear when averaging our conditions (28) which yields

$$(\nabla_{p_j} - \nabla_P) \cdot A_{kj} = 0 \quad (70)$$

In particular, at $k = 1$ the latter formula can be rewritten as

$$\nabla_{u_1} \cdot A_{11} = 0$$

This equality shows, first, that A_{11} has meaning of flow of two-particle (BP-atom) correlations in space of

relative velocity $u_1 = v_1 - V$. Second, this flow is either purely rotational or simply constant vector. Following the “Ockham razor” principle, it is natural to choose the latter variant, since the former one has no visible physical sense (at least in theory where particles do not rotate). Then

$$A_{11} = \oint \Omega Q_1(\rho_1 = a\Omega) = A_{11}(t, R, P + p) ,$$

that is the space angle integral in collision term of the first of Eqs.27, for F_0 , depends on total momentum of colliding pair only.

2, Similar statement can be concluded as true in respect to the function $Q_1(\cdot)$ itself, which characterizes local (R -dependent) rate of (various types of) collisions. Namely,

$$Q_1(\rho_1 = a\Omega) = Q_1(t, R, \Omega, P + p) \quad (71)$$

In other words, rate of collisions depends on centre of mass velocity, $(MV + mv)/(M + m)$ (CMV) only, but not separately on BP’s and atom’s velocities.

Consequently, CMV is characteristic velocity of drift of (mean) collision rate in real configurational space.

3. Analogous discussion of functions

$$B_k = Q_k(\rho_1 = a\Omega_1, \dots, \rho_k = a\Omega_k) \quad (72)$$

and functions $\oint_1 \dots \oint_k \Omega_1 \dots \Omega_k B_k$ (multi-vector, or tensor-like, objects) pushes to suppose that all they depend on momenta or velocities through single variable, $P + p_1 + \dots + p_k$ or, equivalently, $(k + 1)$ -particle CMV $(MV + mv_1 + \dots + mv_k)/(M + km)$. In particular,

$$B_k = B_k(t, R, \Omega_1, \dots, \Omega_k, P + p_1 + \dots + p_k) \quad (73)$$

That are statistical characteristics of randomness, or fluctuations, of collisions’ rate. Although we can interpret them also as characteristics of local rates of specific many-particle configurations and events. Anyway, taking in mind that the particles might belong to either one and the same “coherent” process or to two or several competitive or concurrent processes. Property (73) allows to expect that these characteristics drift with CMVs $(MV + mv_1 + \dots + mv_k)/(M + km)$.

4. These reasonings are in agreement with results of our first analysis of BBGKY hierarchy in [3] in the framework of “collisional as approximation” suggested there (see also [11, 12, 19]). Simply, relative motion of colliding (or close) particles is inner constituent part of their collision (or encounter) and therefore does not contribute to spatial drift of collision (encounter) as the whole which thus acquires centre of mass velocity (CMV).

In the rest of this paper, let us point out how solutions to BBGKY equations are constructed, and why they possess properties like (72)-(73), thus cardinally destroying naive Boltzmann’s molecular chaos, by transmuting its relaxation rates into random quantities. As before, we shall exploit particular example of “BP in ideal gas”, but our reasonings will be quite general.

VII. CHARACTERISTIC STRUCTURE OF SOLUTIONS TO (HARD-BALL) BBGKY HIERARCHY

A. Stationary solutions and Liouville operators

1. First, discuss stationary solutions of Eqs.27 or, equivalently Eqs.33 (or Eq.38), when all $\dot{Q}_k = \dot{C}_k = 0$. Clearly, such solutions must be at once spatially homogeneous: $\nabla_R Q_k = \nabla_R C_k = 0$. Designating them by $Q_k^o = Q_k^o(\rho_1, \dots, P, p_1, \dots)$ and C_k^o , we thus have

$$0 = \sum_{j=1}^k \hat{L}_j Q_k^o + \quad (74)$$

$$+ na^2 \oint dp_{k+1} (\Omega \cdot (v_{k+1} - V)) \times$$

$$\times G_m(p_{k+1}) Q_{k+1}^o(\rho_{k+1} = a\Omega)$$

and similarly for C_k^o , where \hat{L}_j means partial Liouville operator (15) in the hard-ball limit defined by expression $\hat{L}_j = (V - v_j) \cdot \nabla_{\rho_j}$ for $|\rho_j| > a$ and by the CBC at $|\rho_j| = a$, (23) or (28) for Q_k^o ’s and (34) or (35) for C_k^o ’s. One may supply these equations with some boundary conditions at infinity, e.g. $Q_k^o(\rho_j = \infty) = Q_{k-1}^o$ or $C_k^o(\rho_j = \infty) = 0$.

2. Of course, there is trivial solution $Q_k^o = \text{const}$, at $\text{const} = 1$ describing (standardly normalized) canonical thermodynamically equilibrium state of the system, free of any information about BP’s position and inter-particle statistical correlations. Notice that it appears from exact time-dependent solution of Eqs.27, with initial conditions (29), when removing its dependence on BP’s position R by integration over R :

$$\int Q_k dR = 1 , \quad (75)$$

since $\int Q_k(t = 0) dR = 1$. Thus, all mathematical problems induced by Eqs.27 can be killed by the single integration.

We, however, are interested in essence of these problems and, therefore, in question whether there are non-trivial (non-constant) solutions of Eqs.74, i.e. such solutions that, in terms of related cumulant functions (CF) (31), $C_k^o \neq 0$ at $\rho_j \neq \infty$ and $C_k^o \rightarrow 0$ when at least one $\rho_j \rightarrow \infty$. Our principal statement is that such solutions indeed exist.

The point is that any solution to Eqs.74 is nothing but chain of k -dimensional projections of a solution to infinitely many-dimensional Liouville equation

$$[-V \cdot \nabla_R + \sum_{j=1}^N \hat{L}_j] Q_N^o = 0, \quad (76)$$

with large $N \Rightarrow \infty$.

Undoubtedly, at any N this equation has infinitely rich variety of non-constant solutions, both dependent and independent on R . Their peculiarity is that any of them keeps constant (invariant in respect to translations) along phase trajectories of the system, in its $(N+1)$ -particle phase space, but can change along different transversal directions, - i.e. from one trajectory to another, - in arbitrarily irregular way.

For example, we may establish it to be non-zero at such trajectories only on which BP's collisions with several or even all of N atoms definitely take place (sometime or, may be, within a given time interval). Arbitrary linear or nonlinear combination of such or otherwise specified functions of $(N+1)$ -particle phase point belongs to the same class of functions, i.e. eigenfunctions of $(N+1)$ -particle Liouville operator with zero eigenvalue.

By these means, it is possible to compose Q_N^o producing, under $N \rightarrow \infty$, a sequence of standardly connected partial functions Q_k^o ($k = 0, 1, 2, \dots$) representing non-trivial solution to Eqs.74.

By their construction, such Q_k^o ($k = 1, 2, 3, \dots$) must look like *localized excitations* of correlation field [31]. At that, since they are stationary, they possess definite symmetry in respect to time reversal, that is equally include post-collision and pre-collision inter-particle correlations.

Besides, due to high degree of arbitrariness in such constructions, their result Q_k^o 's satisfying Eqs.74 simultaneously can be furnished with an infinite set of free parameters.

3. Spatial extension, in ρ_j -spaces, of the localized excitations is determined by the "collision integrals" in Eqs.74. Naturally, this extension, let be denoted by d , is of order of characteristic BP's "mean free path" $\sim \lambda = (\pi a^2 n)^{-1}$. More precisely, it may depend also on BP-atom relative velocities, since, strictly speaking, this integrals determine sooner characteristic "rate" of BP's collisions, $\sim u_0/\lambda$, - with $u_0 = \sqrt{T/m'}$, $m' = (mM/(m+M))$, - so that

$$d \sim \lambda |v - V|/u_0$$

Then at $|\rho_j| \lesssim d$ one can neglect effect of collisions with outer particles and write approximately

$$\sum_{j=1}^k \hat{L}_j Q_k^o = 0 \quad (77)$$

($k > 0$), instead of (74), with contact boundary values $Q_k^o(|\rho_j| = a)$ considered like "initial conditions" to

$(k+1)$ -particle phase trajectories. Solutions to them as well allow for many free parameters. In particular, total $(k+1)$ -particle momentum $P_k = P + \sum_{j=1}^k p_j$ can be treated as one of parameters, because it is conserved by the Liouville operator there.

B. Quasi-stationary asymptotics of inter-particle correlations

1. Another important statement to argue is that inter-particle correlations, which are induced by BP's walk after start from non-correlated state (29) and described by Eqs.27 or Eqs.33, do not disappear with time, instead going to approximately stationary asymptotics satisfying Eqs.74.

This is clear already from the first of DVR (36) if rewriting it as

$$\frac{\partial \ln Q_0}{\partial \ln n} = n \int_{|\rho_1| > a} \int_{p_1} G_m(p_1) \left[\frac{Q_1}{Q_0} - 1 \right] \quad (78)$$

and taking into account that all Q_k s decrease with time proportionally to Q_0 , - $Q_k \propto Q_0$, - while Q_0 decreases with (long enough) time by a "diffusive law",

$$Q_0(t, R, P | n) \sim (4\pi Dt)^{-3/2} \Psi(R^2/4Dt) \quad (79)$$

Here $D = D(n)$ is characteristic diffusivity, and function $\Psi(\cdot) \geq 0$ ($\Psi(0) = 1$) and generally is not exponential (reducing to exponential at $M/m \rightarrow \infty$ only) [12–15, 17, 19, 22, 24]. For dilute gas, or under BGL $D(n) \sim \lambda \sqrt{T/M} = \sqrt{T/M}/(\pi a^2 n) \propto 1/n$. From Eqs.78 and 79 it follows that at large time ("far at kinetic stage") both sides in Eq.78 become a function of single dimensionless argument $\zeta = R/\sqrt{2Dt}$, that is has non-zero finite limit when $t \rightarrow \infty$ at any fixed ζ or R .

This means, in turn, that ratios Q_k/Q_0 have non-zero long-time limits, moreover, quantities that factors $Q_1/Q_0 - 1$ and $Q_{k+1}/Q_k - 1$, - representing BP-atoms correlations, stay non-zero.

2. Hence, we can identify (accurate to some common positive multiplier) the limit ratios Q_k/Q_0 , on one hand, and the above suggested functions Q_k^o satisfying stationary Eqs.74, on the other hand. At that, Q_k^o acquire argument R , or $\zeta = R/\sqrt{2Dt}$, in the role of free parameter, among other possible ones.

Correspondingly, we can use Eqs.74 or Eqs.77 as a tool for constructing qualitatively correct approximations of actual non-stationary solutions to Eqs.27.

C. Collisional approximation

1. Basing on all the aforesaid, let us try to separate "fine details" of inter-particle correlations, - at small relative distances from $|\rho| \sim a$ up to $|\rho| \sim \lambda$, - and overall value of these correlations varying at larger distances

$|\rho| \gtrsim \lambda$, - by assuming that the first take a constant shape at kinetic stage of evolution, while the second continues to change together with probability distribution of BP's position. The first are correlations inside clusters of close particles conserving their summary momentum $P_k = P + \sum_{j=1}^k p_j$. The second is represented by a set of mean densities of $(k+1)$ -particle clusters in real configurational space.

Naturally, these densities are drifting with the centre-of-mass velocities (CMV) $V_k = P_k/M_k = V + (m/M_k) \sum_{j=1}^k u_j$ (where $M_k = M + km$) and therefore must be "attached" to centre-of-mass position

$$R_k = (MR + m \sum_{j=1}^k r_j)/M_k = R + \frac{m}{M_k} \sum_{j=1}^k \rho_j \quad (80)$$

To separate the latter from relative motion of particles inside clusters, let us rewrite Eqs.27 in the form

$$\begin{aligned} \dot{Q}_k &= -V_k \cdot \nabla_R Q_k + \quad (81) \\ &+ \sum_{j=1}^k [\hat{L}_j + \frac{m}{M_k} u_j \cdot \nabla_R] Q_k + \\ &+ na^2 \oint \Omega \cdot \langle (v - V) Q_{k+1}(\rho_{k+1} = a\Omega, p_{k+1} = p) \rangle_p, \end{aligned}$$

where $p = mv$ and angle brackets denote averaging over equilibrium atom's momentum distribution:

$$\langle \dots \rangle_p = \int \dots G_m(p) dp$$

We thus excluded parts $(m/M_k) u_j \cdot \nabla_R Q_k$ from the first right-hand term and added them to \hat{L}_j . Due to this transfer, evolution operators defined in first and second rows of Eqs.81 now commute one with another, even in respect to spatially inhomogeneous Q_k s, i.e. somehow depending on R (or, equivalently, on R_k s).

2. Hence, we can associate these operators with evolutions of "overall" density of correlated many-particle clusters and "fine" distribution of correlations inside clusters, respectively. Then, - following the claimed course, - assume that at kinetic, or "quasi-stationary", stage of evolution, for relatively close particles, approximately

$$\sum_{j=1}^k [\hat{L}_j + \frac{m}{M_k} u_j \cdot \nabla_R] Q_k = 0 \quad (82)$$

By essence, this is the same equation as Eq.77, with those difference only that, evidently, solutions to Eq.82 possess P_k and R_k among their free parameters, instead of P_k and R for solutions of Eq.77.

Probability-theoretical meaning of Eq.82, as well as Eq.77, is very simple: it states that, in statistical ensemble under consideration, various sequential stages (time

sections) of one and the same two-particle collision, or more complex many-particle event, are represented with equal probabilities (probability densities). Clearly, this is quite necessary condition (ansatz) since otherwise one could not treat a given configuration as time section (instant view) of definite coherent collision or event as the whole.

That is why thus arising approach, for the first introduced in [3], later in [11, 12, 16, 19] was named "collisional approximation". At that, generally, "collisions" are meant in wide sense as chains or packs of connected or competitive ("mutually interfering", "virtual", etc.) or merely close pair collisions, or may be even "encounters" of particles without substantial interaction.

3. In essence, Eqs.77 and 82 serve as direct analogues of the "extended CBC" (4)-(5). To see this, let us apply similar reasonings to events ("multi-particle collisions") associated with specific configurations with all $|\rho_j| \rightarrow a$. Considering them in the centre-of-mass frame, we have, instead of (4),

$$\begin{aligned} F_k \left(R = R_0 + \frac{m}{M_k} \sum u_j dt, \rho = a\Omega - u dt, u \right) &= \quad (83) \\ = F_k \left(R = R_0 - \frac{m}{M_k} \sum u_j^* dt^*, \rho = a\Omega + u^* dt^*, u^* \right) \end{aligned}$$

Here ρ , Ω and u replace full sets of variables, $dt > 0$ and $dt^* > 0$ again are arbitrary infinitesimal quantities, and

$$R_0 \equiv R_k - \frac{m}{M_k} \sum a \Omega_j$$

This condition yields, instead of (5),

$$\left[- \sum u_j \cdot (\nabla_{\rho_j} - \nabla_R) F_k \right]_{|\rho|=a} = 0, \quad (84)$$

which coincides with Eq.82 as applied to vicinity of multiple collision boundary, $\rho_j \rightarrow a\Omega_j$. Such short-cut version of Eq.82, however, is sufficient for deducing the collisional approximation.

4. Since in this approximation we neglect details of distributions of inter-particle correlations in $x = \{\rho, p\}$ -spaces, - when excluding second row of Eqs.81, - we must correspondingly roughen also third row there, by excluding from it now inaccessible "fine" information about momenta and space-angles' dependencies of boundary values of DFs or CFs. More precisely, information about pre-collision correlations between momenta of actually colliding particles (BP and "outer" atom).

To perform this simplification, firstly, let us apply the conventional CBC (23) to express, as usually, the "collision integrals" in Eqs.81 through pre-collision states. Secondly, make there replacement

$$\begin{aligned}
& Q_{k+1}(\rho_{k+1} = a\Omega, p_{k+1} = p) \Rightarrow \\
& \Rightarrow \langle Q_{k+1}(\rho_{k+1} = a\Omega, p_{k+1} = p) \rangle_p \\
& \quad \text{at } (\Omega \cdot (v - V)) < 0
\end{aligned} \tag{85}$$

We thus treat the “outer” (($k+1$)-th) atom like “thermostat atom” whose random momentum just before its collision with BP obeys purely Maxwell distribution. Simultaneously, of course, we have to ignore a questionable “fine” dependence of $Q_{k+1}(\rho_{k+1} = a\Omega, p_{k+1} = p)$ on Ω at $(\Omega \cdot (v - V)) < 0$. It means that we prescribe uniform distribution of the collision’s impact parameter $a[\Omega - u(u \cdot \Omega)/u^2] \perp u$. This ansatz, however, has a little in common with Boltzmann’s “molecular chaos” hypothesis, since in general ratio Q_{k+1}/Q_k , as well as $\langle Q_{k+1} \rangle_p / Q_k$, is different from unit and possesses significant dependence on momenta of all other k atoms.

After all that, one comes to equations

$$\dot{Q}_k = -V_k \cdot \nabla_R Q_k + \hat{B}^\dagger \langle Q_{k+1} \rangle_p, \tag{86}$$

where $Q_k = Q_k(t, R, P, p_1 \dots p_k)$,

$$\begin{aligned}
& \langle Q_{k+1} \rangle_p = \\
& = \int Q_{k+1}(t, R, P, p_1 \dots p_k, p) G_m(p) dp,
\end{aligned} \tag{87}$$

and $\hat{B}^\dagger = \hat{B}^\dagger(V, \nabla_P)$ is conjugated (transposed) Boltzmann-Lorentz operator defined by

$$\begin{aligned}
\hat{B}^\dagger Q(P) &= na^2 \int_p \oint_{(\Omega \cdot (v-V)) < 0} (\Omega \cdot (v - V)) \times \\
&\times G_m(p) [Q(P) - Q(P^*)]
\end{aligned} \tag{88}$$

The latter is connected to the usual Boltzmann-Lorentz operator \hat{B} by operator-valued equality

$$\hat{B} G_M(P) = G_M(P) \hat{B}^\dagger$$

Notice that at $k > 0$ in Eqs.86 the BP’s coordinate vector R in fact plays as the centre-of-mass coordinates R_k , since $\nabla_R R_k = 1$ (besides, R practically coincides with R_k at $|\rho_j|$ s comparable with a).

It should be noticed also that the same shortened Eqs.86 can be easily derived directly from Eqs.27 if considering the boundary DFs (72) and applying the CBC extension in the form e.g. of Eqs.84.

5. The Eqs.86 are equivalent to equations originally deduced in [3]. In spite of presence of the Boltzmann-Lorentz operator in these equations, they predict crucial violation of Boltzmann’s “molecular chaos”, so that certainly

$$\langle Q_{k+1} \rangle_p \neq Q_k$$

In particular, quantity $\langle Q_1 \rangle_p$ there, - which represents local (space-time dependent) ensemble-averaged density,

or probability density, of BP-atom collisions, - does not reduce to quantity Q_0 representing BP’s probability density distribution $F_0 = G_M(P) Q_0$. Instead, both they are determined by all the infinite rest of hierarchy Eqs.86.

Physically, this means that dynamical system under our consideration possesses no *a priori* predictable “probabilities of collisions” which would be same for “almost all” realizations of the system’s dynamical evolution (experiments). Instead, almost all experiments show their own unique *a posteriori* “probabilities” (relative frequencies).

Mathematically, all that is caused by the drift terms in Eqs.86, which state that density distributions of different sorts of collisions (and many-particle events) shift in space with different centre-of-mass drift velocities. Just this is formal source of inter-particle correlations. It shows that correlations arise in spatially inhomogeneous statistical ensembles and, hence, by their nature are spatial correlations. On the other hand, this source appears in the foreground like the “Cheshire Cat’s smile” while the “Cat himself”, that is detail microscopic background picture of the correlations, becomes invisible under the “collisional approximation”.

Some possibilities of this approach were presented in [3, 11, 12, 19]. It qualitatively reveals true statistics of “molecular Brownian motion” and even gives its reasonable semi-quantitative estimates, in particular, for accompanying diffusivity/mobility $1/f$ -noise.

But complete structure of solutions to basic exact BBGKY hierarchies still requires serious mathematical investigation. To end this paper, let us shortly discuss some of related questions.

VIII. BEYOND THE COLLISIONAL APPROXIMATION

A. Localization of inter-particle correlations and space-angle averaging in the Boltzmann-Grad limit

1. When considering ρ_j -dependencies of solutions to Eqs.27 or Eqs.33 or Eqs.74, etc., it seems natural to use spherical coordinates, e.g. in terms of variables

$$q_j = \frac{|\rho_j|}{a}, \quad \Omega_j = \frac{\rho_j}{|\rho_j|},$$

and transformations like

$$Q(\dots \rho_j \dots) \Rightarrow \oint Q(\dots a q_j \Omega \dots) f(\Omega)$$

with proper space angle functions $f(\Omega)$, e.g. in order to extract various “multi-pole components” of ρ_j s dependent fields.

Motivation for such manipulation is obvious: the collision integrals are determined by “dipole” components

at $q_{k+1} = 1$, while the dynamical virial relations (DVR) involve “scalar” components integrated over all q_{k+1} ’s values. For example, Eq.78, if rewritten, once more, via the cumulant functions, as

$$\frac{\partial C_0}{\partial \ln a^2 n} = a^3 n \int_1^\infty dq_1 q_1^2 \int_{p_1} G_m(p_1) \oint C_1 \quad (89)$$

2. The latter formula clearly prompts that under the BGL, when $a^3 n = a/\pi\lambda \rightarrow 0$ (with fixed characteristic free path length $\lambda = (\pi a^2 n)^{-1} = \text{const}$), the scalar component of C_1 behaves like

$$C_1^0 \equiv \frac{1}{4\pi} \oint C_1 \Rightarrow \frac{S_1^0(aq_1/\lambda)}{q_1^2}, = \frac{a^2 S_1^0(|\rho_1|/\lambda)}{|\rho_1|^2} \quad (90)$$

with some integrable function $S_1^0(\cdot)$. Otherwise right-hand side in (89) would have either zero or infinite limit.

Such characteristic law of localization of inter-particle (BP-atom here) correlations, as in (90), can be argued, heuristically or formally, in several different ways [13, 20, 21].

Thus, at short enough relative distances (comparable with a) space angle-averaged inter-particle correlation decreases inversely proportionally to area $4\pi q^2$ of surrounding sphere (similarly to light intensity around point emitter in transparent medium), while at long distances (comparable with λ) the decrease is much more fast (similarly to light in absorbing medium).

Analogously, in the light of other higher-order DVR it is clear that all scalar components of all higher-order CFs must obey, under BGL, the same behavior as in (90):

$$C_k^{0\dots 0} \equiv [\prod_j \frac{1}{4\pi} \oint] C_k \Rightarrow \\ \Rightarrow [\prod_j \frac{a^2}{|\rho_j|^2}] S_k^{0\dots 0}(|\rho_1|/\lambda, \dots |\rho_k|/\lambda) , \quad (91)$$

with $\oint_j \dots = \int d\Omega_j \dots$ and functions $S_k^{0\dots 0}$ scaled by λ independently on $a/\lambda \rightarrow 0$.

3. Further, let us consider dipole components of CFs and show that under BGL their dependence on ρ_j s also takes form like (90) and (91).

From the second of Eqs.33 one has

$$\begin{aligned} \partial_t C_1^0 &= -V \cdot \nabla_R C_1^0 + \\ &+ (V - v_1) \cdot \frac{1}{4\pi} \oint \nabla_{\rho_1} C_1 + \\ &+ \frac{4}{\lambda} \int dp_2 G_m(p_2) (v_2 - V) \cdot C_2^{01}(|\rho_2| = a) , \end{aligned} \quad (92)$$

where

$$C_2^{01} = \frac{1}{4\pi} \oint_1 \frac{1}{4\pi} \oint_2 \Omega_2 C_2 \quad (93)$$

Integral in the second row here can be transformed with the help of general easy provable identity

$$\begin{aligned} &\oint f(\Omega) [-(u \cdot \nabla_\rho) C] = \\ &= -\left(\frac{2}{|\rho|} + \partial_{|\rho|}\right) \oint (u \cdot \Omega) f(\Omega) C + \\ &+ \frac{1}{|\rho|} \oint C (u \cdot [1 - \Omega \otimes \Omega] \cdot \nabla_\Omega) f(\Omega) , \end{aligned} \quad (94)$$

with arbitrary function $C = C(\rho) = C(|\rho|, \Omega)$ and \otimes denoting direct (tensor) product of vectors. It yields

$$\begin{aligned} \partial_t C_1^0 &= -V \cdot \nabla_R C_1^0 - \\ &- \left(\frac{2}{|\rho_1|} + \partial_{|\rho_1|}\right) (u_1 \cdot C_1^1) + \\ &+ \frac{4}{\lambda} \int dp_2 G_m(p_2) (v_2 - V) \cdot C_2^{01}(|\rho_2| = a) , \end{aligned} \quad (95)$$

where the dipole C_1 ’s component appears,

$$C_1^1 = \frac{1}{4\pi} \oint \Omega_1 C_1$$

(which is a vector function, naturally).

Now, we have to discuss possible dependence of this component on $|\rho_1|$ at distance $|\rho_1|$ comparable with a . There we can write $C_1^1 = C_1^1(|\rho_1|/a)$, with $C_1^1(1)$ staying finite under BGL, of course. Evidently, then second-row expression in Eq.95 stays finite too if and only if

$$\left[\frac{2}{q_1} + \partial_{q_1}\right] C_1^1(q_1) = 0$$

(otherwise it would tend to infinity $\propto \lambda/a$). This just means that on the whole

$$C_1^1 \Rightarrow \frac{S_1^1(aq_1/\lambda)}{q_1^2} = \frac{a^2}{|\rho_1|^2} S_1^1(|\rho_1|/\lambda) , \quad (96)$$

similarly to (90) (simultaneously, this is confirmation of the BGL asymptotics (90)).

Hence, Eq.95 turns, - after multiplying it by q_1^2 and going to BGL, - into

$$\begin{aligned} \partial_t S_1^0 &= -V \cdot \nabla_R S_1^0 - \partial_{|\rho_1|} (u_1 \cdot S_1^1) + \\ &+ \frac{4}{\lambda} \int dp_2 G_m(p_2) (v_2 - V) \cdot S_2^{01}(|\rho_2| = 0) , \end{aligned} \quad (97)$$

where, clearly, $S_2^{01} = q_1^2 q_2^2 C_2^{01}$.

4. Next, let us discuss evolution equations for C_1^1 and similar dipole or “multi-dipole” components of higher-order CFs.

Applying the identity (94), with $f(\Omega) = \Omega$, to some of the space angles, one easily obtains

$$\begin{aligned} & \frac{1}{4\pi} \oint \Omega [-(u \cdot \nabla_\rho) C] = \\ & = -\frac{1}{3} u \partial_{|\rho|} C^0 - \left[\frac{3}{|\rho|} + \partial_{|\rho|} \right] (C^2 \cdot u) , \end{aligned} \quad (98)$$

where, as above, C^0 symbolizes scalar component of $C = C(|\rho|, \Omega)$ (in respect to given space angle), while C^2 its “quadrupole” component as defined by

$$C^2 = \frac{1}{4\pi} \oint [\Omega \otimes \Omega - \frac{1}{3}] C \quad (99)$$

(thus it is tensor quantity).

In view of what we already know about behavior of scalar and dipole C_k ’s components under BGL, it is obvious that differentiation in the first right-hand term in (98) produces extra factor $\propto \lambda/|\rho| \sim \lambda/a$ which tends to infinity and therefore must be compensated by proper contribution from the second term. The latter, besides, should not produce its own such factor. These requirements mean that the quadrupole component (99) looks like

$$C^2 = \frac{a^2}{|\rho|^2} S^2 + \frac{a^3}{|\rho|^3} U^2 , \quad (100)$$

where $S^2 = S^2(|\rho|/\lambda)$ and $U^2 = U^2(|\rho|/\lambda)$ are scaled by BP’s free path (or other value insensitive to BGL), and S^2 is related to S^0 by condition

$$S^2 = \frac{2}{3} S^0 + \left[\frac{u \otimes u}{|u|^2} - 1 \right] S^{0'} , \quad (101)$$

which just ensures finiteness of the expression (98) at $a/\lambda \rightarrow 0$ and $|\rho|$ comparable with a .

Then, notice that actually the second term in (100) must have zero value, i.e. $U^2 = 0$, since otherwise scalar and dipole components of CFs also would acquire, - through Eqs.33, - contributions $\propto a^3/|\rho_j|^3$, which however certainly are forbidden by our previous analysis. Besides, factual contribution to C^2 from the second term of (101) equals to zero (merely by definition of this term).

Due to these reasons, we find from (98), (100) and (101) that expression (98) reduces simply to

$$\begin{aligned} & \frac{1}{4\pi} \oint \Omega [-(u \cdot \nabla_\rho) C] = \\ & = -u \frac{a^2}{|\rho|^2} \partial_{|\rho|} S^0 \end{aligned} \quad (102)$$

Consequently, equations of evolution of C_k ’s dipole components involve respective C_k ’s scalar components only. In particular, we have

$$\begin{aligned} & \partial_t S_1^1 = -V \cdot \nabla_R S_1^1 - u_1 \partial_{|\rho_1|} S_1^0 + \\ & + \frac{4}{\lambda} \int dp_2 G_m(p_2) (v_2 - V) \cdot S_2^{11}(|\rho_2| = 0) \end{aligned} \quad (103)$$

Similarly, evolution of higher-order “multi-scalar-dipole” C_k s components,

$$S_k^{\sigma_1 \dots \sigma_k} \quad (\sigma_j = 0, 1) ,$$

involves the same set of functions only, with various “scalar-dipole” superscript replacements $\sigma_j \Leftrightarrow 1 - \sigma_j$, plus half of analogous next-order set, $S_{k+1}^{\sigma_1 \dots \sigma_k 1}$.

5. Introducing column 4-vector $S_1 = \{S_1^0, S_1^1\}$, we can unify Eqs.97 and 103 into

$$\begin{aligned} & \partial_t S_1 = -V \cdot \nabla_R S_1 - U_1 \partial_{|\rho_1|} S_1 + \\ & + \frac{4}{\lambda} \int dp_2 G_m(p_2) \{0, u_2\}^\dagger \cdot S_2(|\rho_2| = 0) , \end{aligned} \quad (104)$$

with 4×4 -matrix

$$U_1 = \left\{ \begin{array}{cc} 0 & u_1^\dagger \\ u_1 & 0 \end{array} \right\} ,$$

symbol \dagger denoting vector or matrix transposition, and row 4-vector $\{0, u_2\}^\dagger$ associated with “outer” atom.

Quite similarly, all 2^k scalar and dipole components $S_k^{\sigma_1 \dots \sigma_k}$ can be unified into single $4 \times \dots \times 4$ -tensor object S_k , and then all evolution equations for these components replaced by more compact hierarchy of equations for tensors S_k which trivially generalize Eq.104.

6. Thus, it seems that Eq.104 altogether with its just mentioned higher-order analogues (plus first of Eqs.33 for $S_0 \equiv C_0$) form a closed (although infinite) system of equations.

In fact, however, situation is not so comfortable. The matter is that at the same time the collision boundary conditions (CBC), (34) or (35), in general involve also S_1^2 and various other quadrupole and multi-pole components of BP-atoms correlations (corresponding to $\sigma_j = 2, 3, \dots$). For example, at $k = 1$ our CBC (35), after its multiplying by $f(\Omega_1) = 1$ or $f(\Omega_1) = \Omega_1$ and space-angle averaging produces

$$(\nabla_{p_1} - \nabla_P) \cdot S_1^1(|\rho_1| = 0, P, p_1) = 0 , \quad (105)$$

$$\begin{aligned} & \frac{1}{3} (\nabla_{p_1} - \nabla_P) [S_1^0(|\rho_1| = 0, P, p_1) + S_0(P)] + \\ & + (\nabla_{p_1} - \nabla_P) \cdot S_1^2(|\rho_1| = 0, P, p_1) = 0 , \end{aligned} \quad (106)$$

where $S_0 = C_0$, and we took into account our above analysis. At that, there are no evident formal reasons to exclude second term of expression (101), e.g. assuming $S_1^{0'} = 0$, and thus reduce S_1^2 to S_1^0 .

Hence, in contrast to evolution equations themselves, the CBC they require are not closed in respect to scalar and dipole CF's components, even under BGL.

Nevertheless, just presented consideration may be base for a meaningful approximation in Eq.106 and similar CBC and thus for approximate solution of Eqs.33.

All that is interesting subject for separate discussion. Here, we at least illustrated by one more method that BGL does not "lighten" the problems of gas kinetics. They remain, again resembling "Cheshire Cat's smile".

B. Pseudo-Liouville representation of hard-ball dynamics

1. In this representation of the conventional theory (see e.g., [2]) the CBC (23) are directly inserted into Liouville operator in the form of singular "interaction" term. In application to our particular system "BP+atoms" this formal trick means that

$$\hat{L}_x \Rightarrow -u \cdot \nabla_\rho + a^2 \oint \delta(\rho - a\Omega) (\Omega \cdot u) \hat{S}(\Omega, P, p), \quad (107)$$

where, as above, $u = v - V$, and $\hat{S}(\Omega, P, p)$ is operator defined by

$$\begin{aligned} \hat{S}(\Omega, P, p) F(P, p) &= \\ &= \theta(-\Omega \cdot u) F(P, p) + \theta(\Omega \cdot u) F(P^*, p^*) \end{aligned} \quad (108)$$

Here $\theta(\cdot)$ is Heaviside step function, and P^* and p^* are pre-collision momenta corresponding to post-collision P and p in accordance with relations (1)-(2). At that, the relative distance ρ formally gets rights to take values from physically forbidden regions, while

$$g(x) \Rightarrow \theta(|\rho| - a) G_m(p)$$

Inserting expression (107) into Eqs.43 and 45, we obtain related generating-functional evolution operators $\hat{\mathcal{L}}$ and $\hat{\mathcal{L}}'$. They are equivalent to full hard-ball BBGKY hierarchy considered in terms of DFs F_k and CFs C_k , respectively.

2. One of formally significant differences of this approach to hard-ball limit from above discussed case of smooth interaction is that now $\hat{\mathcal{L}}'$ contains non-zero $\psi(x)$ -independent part, in contrast to (45). Concretely,

$$\begin{aligned} \hat{\mathcal{L}}' \{V, \psi = 0, \nabla_P, \delta/\delta\psi = 0\} &= \\ &= \int_x n \hat{L}_x g(x) = \hat{B} \neq 0, \end{aligned} \quad (109)$$

where \hat{B} is already mentioned Boltzmann-Lorentz operator (BLO). Now, according to (107) and (108), its action is described by

$$\begin{aligned} \hat{B} &\Rightarrow n a^2 \int_p \oint (\Omega \cdot u) \times \\ &\times [\hat{S}(\Omega, P, p) - 1] G_m(p), \quad (110) \\ \hat{B} F(P) &= n a^2 \int_p \oint (\Omega \cdot u) \theta(\Omega \cdot u) \times \\ &\times [G_m(p^*) F(P^*) - G_m(p) F(P)] \end{aligned}$$

Formally, this part of $\hat{\mathcal{L}}'$ results from the lower-order terms of the hard-ball collision boundary conditions (CBC), Eq.34 (Eq.13 in [6]), as clearly shows the integrand expression in Eq.17 in [6].

C. Pseudo-kinetic representation of hard-ball dynamics

1. Physically, the BLO part of $\hat{\mathcal{L}}'$ can be interpreted as representative of equilibrium thermostat consisting of particles (atoms) uncorrelated with our "Brownian particle" (BP) under observation. Separating this part evidently, let us write

$$\begin{aligned} \hat{\mathcal{L}}' &= \hat{B} + \hat{\mathcal{L}}^+ + \hat{\mathcal{L}}^-, \quad (111) \\ \hat{\mathcal{L}}^+ &\equiv \int_x \psi(x) \hat{L}_x g(x) \end{aligned}$$

Here, we separated also $\hat{\mathcal{L}}'$'s component $\hat{\mathcal{L}}^+$ which rises $\psi(x)$ -dependence of an operand (like "creation operator", in the sense of [16, 24]), while two components of $\hat{\mathcal{L}}^-$, - namely,

$$\begin{aligned} \hat{\mathcal{L}} &= \hat{\mathcal{L}}_0 + \hat{\mathcal{L}}^-, \quad (112) \\ \hat{\mathcal{L}}_0 &\equiv \int_x \psi(x) \hat{L}_x \frac{\delta}{\delta\psi(x)}, \quad \hat{\mathcal{L}}^- \equiv n \int_x \hat{L}_x \frac{\delta}{\delta\psi(x)}, \end{aligned}$$

- respectively conserve this dependence on $\psi(x)$ and lower it (like "annihilation operator").

Then, evolution equation for CF's generating functional (GF) can be rewritten as

$$\partial_t \mathcal{C} = [-V \cdot \nabla_R + \hat{B} + \hat{\mathcal{L}}^+ + \hat{\mathcal{L}}^-] \mathcal{C}, \quad (113)$$

with the same initial condition (50), as before, and same relation to BP's probability distribution function,

$$F_0(t, R, P) = \mathcal{C}\{\psi = 0\}$$

2. If random walk of hard-ball BP obeyed Boltzmann's molecular chaos, then the generating-functional part of evolution operator in Eq.113, - i.e. two last terms of

(111), - would have no effect onto $F_0(t, R, P)$ at least in BGL. In order to highlight the question, - is it really so or not, - it is convenient again to represent Eq.113, - along with equivalent Eq.48 for \mathcal{F} , - via “pseudo-kinetic” operators.

Evidently, such transform by itself does not differ from what we made in case of smooth interaction potential. Therefore, repeating derivation of Eqs.53-55, we again can write

$$\partial_t \mathcal{C} = -V \cdot \nabla_R \mathcal{C} + \hat{\mathcal{K}}'(t) \mathcal{C} , \quad (114)$$

with “pseudo-kinetic” operator (PKO)

$$\begin{aligned} \hat{\mathcal{K}}'(t) &= \int_x [n + \psi(x)] \hat{L}_x \times \\ &\times \exp[(\hat{L}_x + \hat{\mathcal{L}}'_R) t] g(x) \exp[-\hat{\mathcal{L}}'_R t] \end{aligned} \quad (115)$$

or, equivalently,

$$\begin{aligned} \hat{\mathcal{K}}'(t) &= \int_x [n + \psi(x)] \hat{L}_x g(x) + \\ &+ \int_x [n + \psi(x)] \hat{L}_x \int_0^t d\tau \times \\ &\times \exp[(\hat{L}_x + \hat{\mathcal{L}}'_R) \tau] \hat{L}_x g(x) \exp[-\hat{\mathcal{L}}'_R \tau] \end{aligned} \quad (116)$$

Here, as before, $\hat{\mathcal{L}}'_R = -V \cdot \nabla_R + \hat{\mathcal{L}}'$. Notice that in the last transition from Eq.115 to Eq.116, in contrast to transition from Eq.54 to Eq.55, we have not removed term $n \int_x \hat{L}_x g(x)$, since now, - according to Eq.109, - it does not turn to zero.

The latter formula can be rewritten also as

$$\begin{aligned} \hat{\mathcal{K}}'(t) &= \hat{B} + \hat{\mathcal{L}}^+ + \\ &+ \int_x [n + \psi(x)] \hat{L}_x \int_0^t d\tau \times \\ &\times \exp[(\hat{L}_x + \hat{\mathcal{L}}'_R) \tau] \hat{L}_x g(x) \exp[-\hat{\mathcal{L}}'_R \tau] , \end{aligned} \quad (117)$$

- to be combined with Eqs.111 and 112.

Then, solution of Eq.114, in respect to BP's marginal distribution, can be represented by

$$\begin{aligned} F_0(t, R, P) &= \\ &= \left\langle \overline{\exp} \int_0^t [-V \cdot \nabla_R + \hat{\mathcal{K}}'(t')] dt' \right\rangle \times \\ &\times F_0(0, R, P) , \end{aligned} \quad (118)$$

where angle brackets mean, as before, statistical average over ensemble of dynamical trajectories of the system (BP + gas) weighted by equilibrium distribution of initial gas microstates. In our designations,

$$\langle \dots \rangle = [\dots]_{\psi=0}$$

In the language of quantum field theory [16, 24]), this is “vacuum average” $\langle 0 | \dots | 0 \rangle$, or amplitude of vacuum-vacuum transition, where role of “vacuum” is played by gas equilibrium.

D. Failure of Boltzmannian kinetics under hard-ball Boltzmann-Grad limit

1. The last two right-hand terms in Eq.117 represent contribution to BP's kinetics from gas correlations with BP's random walk. In general, undoubtedly, they give substantial addition to the Boltzmann's term \hat{B} , both in the sense of ensemble average and fluctuations of BP's relaxation rates (“friction”, “diffusivity”, “mobility”, etc.). Therefore, let us go to BGL.

This purpose again can be achieved with the help of scale transformation like (60), namely,

$$n \Rightarrow \frac{n}{\xi^2} , \quad a \Rightarrow \xi a , \quad (119)$$

where $\xi \rightarrow 0$, - with $a \Rightarrow \xi a$ applied in the singular “collision” term of pseudo-Liouville operator (107), - supplemented by the same changes of variables $x = \{\rho, p\}$, $\psi(x)$ and τ as in (61), and same transformation of the variational derivative as in (62).

At that, at $\xi \rightarrow 0$ we have $\hat{L}_x \Rightarrow \xi^{-1} \hat{L}_x$, and operators $\hat{\mathcal{L}}$ (112) and $\hat{\mathcal{L}}'$ (111) transform asymptotically exactly as in Eq.63. Consequently, we come to

$$\begin{aligned} \hat{\mathcal{K}}'(t) &\Rightarrow \hat{\mathcal{K}}_\infty = \hat{B} + \hat{\mathcal{L}}^+ + \\ &+ \int_x [n + \psi(x)] \hat{L}_x \int_0^\infty d\tau \times \\ &\times \exp[(\hat{L}_x + \hat{\mathcal{L}}) \tau] \hat{L}_x g(x) \exp[-\hat{\mathcal{L}} \tau] \end{aligned} \quad (120)$$

Hence, the exact pseudo-kinetic operator does not reduce to Boltzmann-Lorentz operator (BLO) even under Boltzmann-Grad limit (BGL).

Let us show that same statement is true also in respect to result of statistical averaging in the exact Eq.65 following from Eq.118 under BGL, that in respect to actual statistics of random walk of our Brownian particle (BP).

2. Basing on logical necessity of correspondence between cases of hard-ball and smooth interactions, we expect that now also on average

$$\langle \hat{\mathcal{K}}_\infty \rangle = \hat{B} ,$$

that is average value of the integral term in Eq.117 equals to zero. It is really so.

Indeed, since action of $\hat{\mathcal{L}}$ onto any $\psi(x)$ -independent object produces zero, we have

$$\langle \hat{\mathcal{K}}_\infty \rangle = \hat{B} + n \int_0^\infty d\tau \int_x \hat{L}_x e^{\hat{\mathcal{L}} \tau} \hat{L}_x g(x)$$

The integral here by its exterior looks like in the “smooth case”, but now its contents represents not a single BP-atom collision but two consecutive BP's collisions with one and the same atom. Since such event is kinematically

impossible, we can state that this integral is equal to zero, and therefore $\langle \hat{\mathcal{K}}_\infty \rangle = \hat{B}$.

3. Next, consider variance of the limit pseudo-kinetic operator $\hat{\mathcal{K}}_\infty$.

Evidently, first, we can write

$$\langle (\hat{\mathcal{K}}_\infty - \langle \hat{\mathcal{K}}_\infty \rangle)^2 \rangle = \quad (121)$$

$$= \left\langle n \int_x \hat{L}_x \int_0^\infty d\tau e^{(\hat{L}_x + \hat{L})\tau} \hat{L}_x g(x) e^{-\hat{L}\tau} \hat{L}^+ \right\rangle$$

Second, in expansion of the exponentials there over “annihilation operator” \hat{L}^- , according to expansion (112), only first-order term survives after averaging, so that

$$\langle (\hat{\mathcal{K}}_\infty - \langle \hat{\mathcal{K}}_\infty \rangle)^2 \rangle = n \int_x \hat{L}_x \int_0^\infty d\tau \int_0^\tau d\eta \times \quad (122)$$

$$\times \langle [e^{\hat{L}_x(\tau-\eta)} \hat{L}^- e^{(\hat{L}_x + \hat{L}_0)\eta} \hat{L}_x g(x) e^{-\hat{L}_0\tau} - e^{\hat{L}_x\tau} \hat{L}_x g(x) \hat{L}^- e^{-\hat{L}_0\eta}] \hat{L}^+ \rangle$$

Third, substituting there \hat{L}^- , \hat{L}_0 and \hat{L}^+ from (112) and (111), we come to visually same expression as in (66). For convenience, we write out it repeatedly:

$$\langle (\hat{\mathcal{K}}_\infty - \langle \hat{\mathcal{K}}_\infty \rangle)^2 \rangle = n^2 \int_x \int_y \int_0^\infty d\tau \int_0^\infty d\tau' \times \quad (123)$$

$$\times \hat{L}_x [e^{\hat{L}_x\tau} \hat{L}_y e^{(\hat{L}_x + \hat{L}_y)\tau'} \hat{L}_x e^{-\hat{L}_y(\tau+\tau')} - e^{\hat{L}_x(\tau+\tau')} \hat{L}_x \hat{L}_y e^{-\hat{L}_y\tau'}] \hat{L}_y g(y) g(x)$$

Its difference from (66) is determined by that of singular pseudo-Liouville \hat{L}_x (107) from “smooth” Liouville operator (44).

4. Figuratively speaking, each of most left or most right-hand of operators \hat{L}_x and \hat{L}_y in Eq.66 is responsible for end or beginning of same collision, respectively, i.e. “half of collision”. What is for Eq.123, in opposite, one can say that there each of these operators represents complete separate collision, since the singular δ -function part of pseudo-Liouville operator (107) by itself makes it.

Under such treatment, second and third rows in Eq.123 describe two variants of four BP’s collisions with two atoms.

At that, clearly, events corresponding to the third row in fact can not realize, by the same kinematic reasons by which the above considered integral in $\langle \hat{\mathcal{K}}_\infty \rangle$ turns to zero. Namely, because two directly consecutive collisions between (mutually repulsing) particles are impossible.

Therefore, we can remove the third row and rewrite Eq.123 simply as

$$\langle (\hat{\mathcal{K}}_\infty - \langle \hat{\mathcal{K}}_\infty \rangle)^2 \rangle = n^2 \int_x \int_y \int_0^\infty d\tau \int_0^\infty d\tau' \times \quad (124)$$

$$\times \hat{L}_x e^{\hat{L}_x\tau} \hat{L}_y e^{(\hat{L}_x + \hat{L}_y)\tau'} \hat{L}_x e^{-\hat{L}_y(\tau+\tau')} \hat{L}_y g(y) g(x)$$

Formally, this expression corresponds to four alternate BP’s collisions with two atoms (described by $x = \{\rho_x, p_x\}$ and $y = \{\rho_y, p_y\}$). The alternation is important there, because just it makes such events kinematically allowed and possible.

Moreover, alternation ensures kinematic and dynamic possibility of arbitrary large number of collisions between BP and two atoms, and such complicated events also are covered by Eqs.115-117, due to presence of the singular \hat{L}_x ’s and \hat{L}_y ’s parts, - in the role of “kinetic operators”, - in the exponentials there.

Hence, we can state that the operator variance (123)-(124) is not zero. This means that Boltzmannian kinetics fails, and the exact kinetic (“pseudo-kinetic”) operator stays different from the Boltzmann’s one and random even in case of hard-ball interaction even under BGL!

This follows also from the “correspondence principle” and above similar statement for arbitrary (in particular, arbitrarily sharp) smooth interaction.

5. Physically, however, too literal treatment of Eqs.115-117 in terms of multiple collisions is rather incorrect.

We should not forget that integrand there is nothing but (second-order) statistical moment of random (operator-valued) quantity.

Therefore seemingly repeated collisions by essence may belong to different “stories”, each without repetitions, with physically different particles. At that, repetitions are merely synonyms of kinematic and dynamical intersections between possible variants of system’s evolution. This is seen from the seed form (115) of the limit pseudo-kinetic operator (120), which displays just interference of current collision in microstate evolution of the rest of gas, or, reciprocally, interference of the latter in realization of the former.

Though, on the other hand, repeated (alternated) collisions and multiply repeated ones in hard-ball systems is their immanent specificity, supported by zero duration of individual collision. Therefore, to some extent, they play role of “smooth” time-stretched collisions. Under such interpretation, for example, the expression inside angle brackets in Eq.121 says about influence of the system’s history, i.e. past collisions, on “probability” of present realization of (alternated) repeated collision.

IX. CONCLUSION

1. Main goal of this manuscript was, firstly, new demonstration, in several original ways, of that the Boltzmann-Grad limit (BGL) does not eliminate effects of inter-particle statistical correlations and therefore does not lead to the Boltzmann’s kinetics. Secondly, this statement equally relates to cases of smooth potential interactions between particles and the hard-ball interaction.

The correlations do their work though surviving at

zero-measure phase-space subsets only, like “angels on needle tip”.

2. In this sense, BGL does not exist. In fact, it results in a non-trivial non-Boltzmannian kinetics which depends on parameter $\pi a^2 n = \lambda^{-1}$ as the whole only, - with a , n and λ denoting interaction radius, mean number density of particles and characteristic free-flight length, - but not on a or n separately (in presence of different sorts of particles, another essential parameters may be their mass, radius and density ratios).

At that, statistics of random walk of a probe “Brownian” particle (BP) is exactly governed by random “pseudo-kinetic” operator (PKO) which takes place of Boltzmann or Boltzmann-Lorentz kinetic operator and coincides with it (under BGL) on average only.

3. Randomness (fluctuations) of the PKO reflects hugeness of number of system’s initial microstate parameters (variables) determining BP’s walk, as compared with number of parameters characterizing this walk.

Importance of giant difference between these numbers already was pointed out in [12, 17] and other our works. It implies impossibility of time averaging of BP’s relaxation rate, i.e. relative frequency and efficiency of its collisions. All the more, because the difference even grows with observation time (and, moreover, turns to infinity under BGL). In other words, it implies non-ergodicity of kinetic properties of “molecular Brownian motion” [17].

As the consequence, diffusivity and mobility of BP possess no a priori certain value, instead changing unpredictably from one experiment, - that is realization of BP’s walk, - to another. Equivalently, we can say that diffusivity (mobility) undergoes scaleless low-frequency fluctu-

ations like 1/f-noise (see references above). Randomness of the PKO just produces such kind of fluctuations

4. So crucial disagreement between our conclusions and that of the pure mathematical analysis of hard-ball gas under BGL in [1, 2] (and earlier in [32]) is not surprising: as we underlined in the body of this manuscript, our consideration concerns events involving finite number of particles but arising in virtually active background of infinitely many other particles, while mathematicians consider events with literally finite particles’ numbers.

To some extent, this resembles quantum mechanics with and without physical vacuum (and such analogy is quite meaningful, since statistical-mechanical problems under our attention indeed can be reformulated in terms of quantum field theory [16, 24, 30]).

Besides, mathematicians filter events by estimates and reasonings based on a priori Lebesgue measures, while our approaches reveal a posteriori significant events (confirming sentence “real is improbable”).

Of course, our theory needs in more formal rigor. At the same time, in our opinion, mathematical theory needs in principal improvements, - in order to become closer to physics, - at that taking into account the Krylov’s criticism [4] and getting rid of ancient prejudices of Boltzmannian kinetics.

5. In the framework of our theory, now new question appears - about inter-relations between earlier suggested approaches to 1/f-noise in diffusivities (mobilities), as well as other relaxation rates, and presently suggested method of the exact random pseudo-kinetic operator. This is one more interesting task for future.

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